



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:30 PM UTC

PDB ID : 3I6S / pdb_00003i6s
Title : Crystal Structure of the plant subtilisin-like protease SBT3
Authors : Rose, R.; Ottmann, C.
Deposited on : 2009-07-07
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

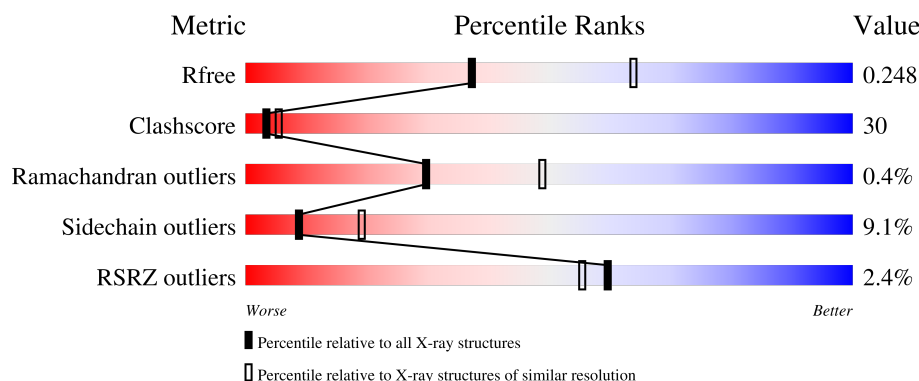
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



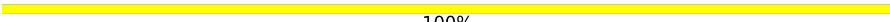
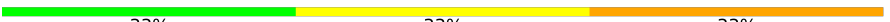
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	649	3% 58% 35% 6%
1	B	649	2% 60% 33% 5%
2	C	2	100%
3	D	3	33% 67%
3	E	3	67% 33%

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Mol	Chain	Length	Quality of chain
3	G	3	 100%
3	H	3	 33% 33% 33%
4	F	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	G	1	-	-	X	-
3	NAG	G	3	-	-	X	-
4	NAG	F	1	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10372 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Subtilisin-like protease.

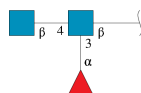
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			4844	3057	833	933	21			
1	B	639	Total	C	N	O	S	0	0	0
			4822	3047	830	924	21			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	G	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	H	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			24	14	1	9			

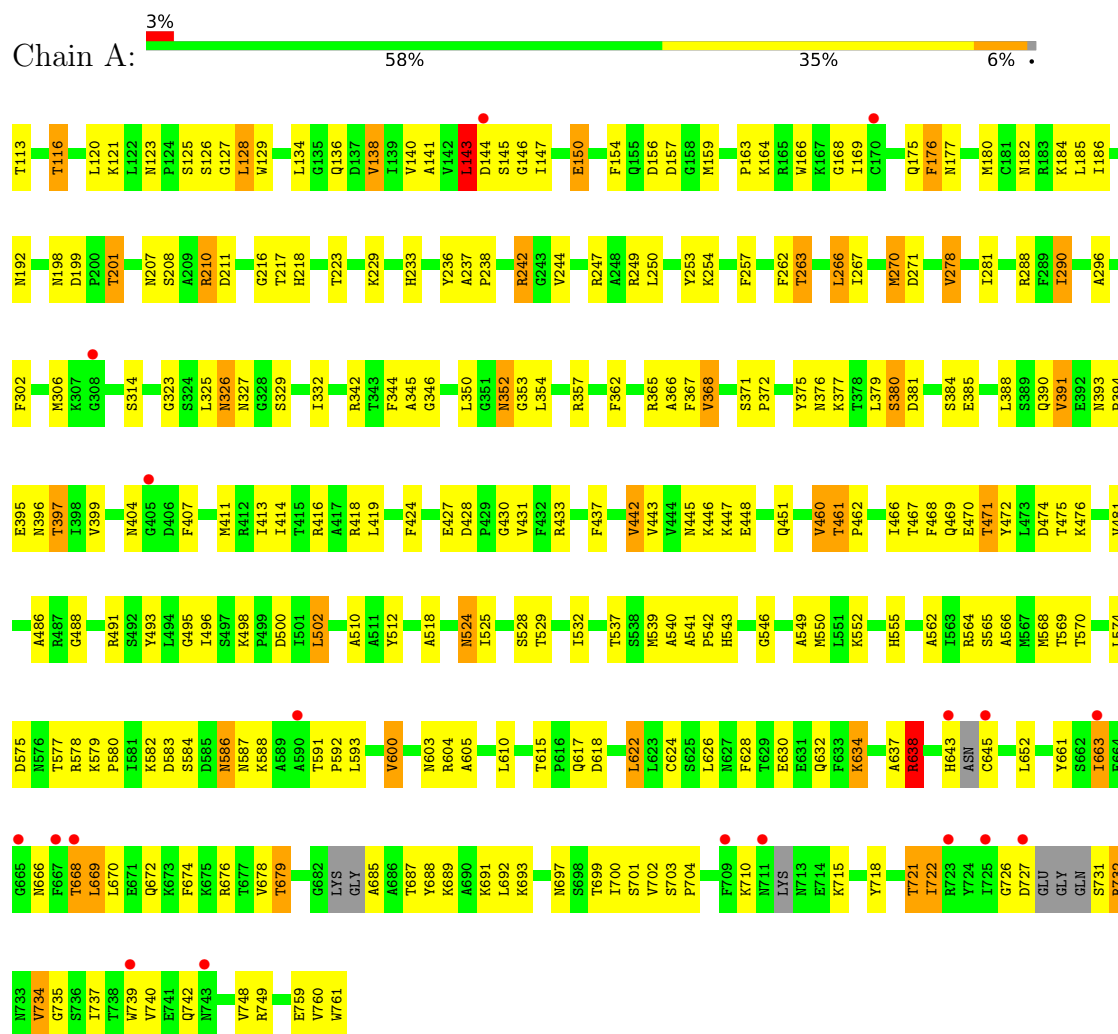
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	212	Total	O	0	0
			212	212		
5	B	290	Total	O	0	0
			290	290		

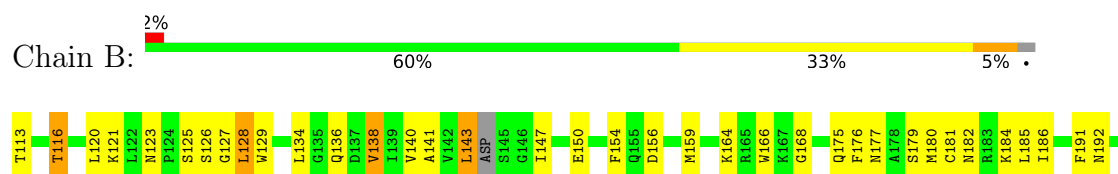
3 Residue-property plots

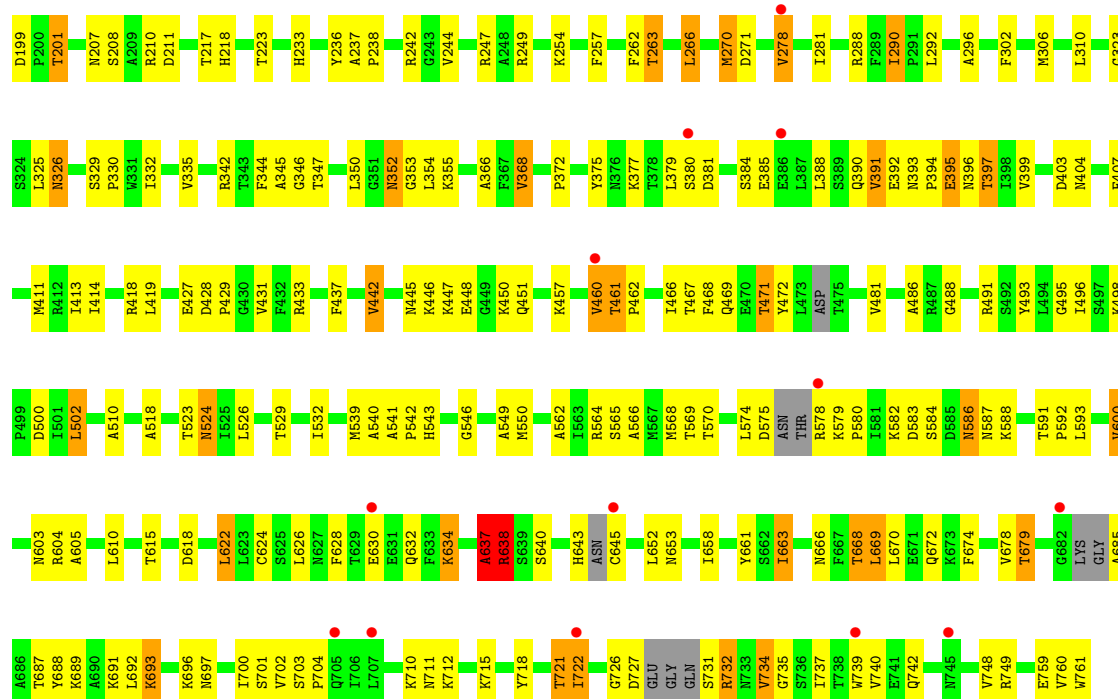
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Subtilisin-like protease



• Molecule 1: Subtilisin-like protease





- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 100%



- Molecule 3: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 33% 67%



- Molecule 3: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 67% 33%



- Molecule 3: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 100%

MAG1
FUC2
MAG3

- Molecule 3: α -L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 33% 33% 33%

MAG1
FUC2
MAG3

- Molecule 4: α -L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%

MAG1
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	143.89Å 143.89Å 195.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.50 19.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.50) 99.7 (19.99-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 2.41Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.249 , 0.283 0.247 , 0.248	Depositor DCC
R_{free} test set	4014 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10372	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FUC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	1/4951 (0.0%)	0.78	1/6737 (0.0%)
1	B	0.38	0/4927	0.79	3/6699 (0.0%)
All	All	0.39	1/9878 (0.0%)	0.79	4/13436 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	PHE	C-N	-5.38	1.25	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	638	ARG	N-CA-C	-9.85	100.50	111.14
1	A	145	SER	N-CA-C	-6.72	105.41	112.93
1	B	637	ALA	N-CA-C	5.85	120.26	113.18
1	B	335	VAL	N-CA-C	5.25	115.86	108.36

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	LEU	Peptide
1	A	210	ARG	Sidechain
1	A	637	ALA	Peptide
1	B	637	ALA	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4844	0	4783	297	0
1	B	4822	0	4773	273	0
2	C	28	0	25	2	0
3	D	38	0	34	1	0
3	E	38	0	33	8	0
3	G	38	0	35	14	1
3	H	38	0	34	1	0
4	F	24	0	22	3	0
5	A	212	0	0	47	1
5	B	290	0	0	44	0
All	All	10372	0	9739	589	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (589) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:THR:HA	5:A:781:HOH:O	1.35	1.25
1:A:475:THR:HA	5:A:908:HOH:O	1.35	1.22
1:B:395:GLU:HG3	5:B:9:HOH:O	1.40	1.18
1:A:591:THR:HG22	1:A:593:LEU:H	1.05	1.17
1:A:674:PHE:HE2	1:A:722:ILE:CD1	1.57	1.17
1:B:674:PHE:HE2	1:B:722:ILE:CD1	1.57	1.16
1:B:591:THR:HG22	1:B:593:LEU:H	1.05	1.15
1:B:674:PHE:CE2	1:B:722:ILE:HD11	1.82	1.14
1:B:591:THR:HG23	1:B:592:PRO:HD2	1.28	1.13
1:A:591:THR:HG23	1:A:592:PRO:HD2	1.22	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:PHE:CE2	1:A:722:ILE:HD11	1.84	1.12
1:B:143:LEU:HD21	1:B:270:MET:HG2	1.32	1.11
1:A:144:ASP:HB3	1:A:146:GLY:H	1.12	1.10
1:A:143:LEU:HD21	1:A:270:MET:HG2	1.31	1.09
1:A:674:PHE:HE2	1:A:722:ILE:HD11	1.13	1.09
1:A:433:ARG:HD2	5:A:854:HOH:O	1.53	1.08
1:B:674:PHE:HE2	1:B:722:ILE:HD11	1.10	1.07
1:A:267:ILE:HG22	5:A:76:HOH:O	1.56	1.05
1:A:679:THR:HG22	5:A:52:HOH:O	1.55	1.04
1:A:674:PHE:CE2	1:A:722:ILE:CD1	2.39	1.03
1:B:375:TYR:HD2	5:B:821:HOH:O	1.38	1.03
1:B:393:ASN:O	1:B:397:THR:HG22	1.58	1.03
1:B:674:PHE:CE2	1:B:722:ILE:CD1	2.38	1.03
1:A:393:ASN:O	1:A:397:THR:HG22	1.59	1.02
1:B:693:LYS:HD2	5:B:977:HOH:O	1.58	1.01
1:A:689:LYS:HD2	1:A:742:GLN:CD	1.86	1.01
1:B:689:LYS:HD2	1:B:742:GLN:CD	1.85	1.00
1:B:721:THR:HG22	5:B:784:HOH:O	1.64	0.95
1:B:177:ASN:H	1:B:180:MET:HE2	1.30	0.94
1:A:638:ARG:HD3	5:A:812:HOH:O	1.69	0.92
1:A:591:THR:CG2	1:A:592:PRO:HD2	2.00	0.92
1:A:591:THR:HG23	1:A:592:PRO:CD	2.00	0.92
1:A:177:ASN:H	1:A:180:MET:HE2	1.35	0.92
1:A:672:GLN:HG2	1:A:674:PHE:CZ	2.05	0.92
1:A:555:HIS:CD2	5:A:878:HOH:O	2.23	0.91
1:B:461:THR:O	1:B:461:THR:HG22	1.70	0.91
3:G:1:NAG:H62	3:G:3:NAG:C1	2.00	0.91
1:A:175:GLN:O	1:A:210:ARG:NH1	2.04	0.90
3:G:1:NAG:H62	3:G:3:NAG:O7	1.69	0.90
1:B:591:THR:CG2	1:B:592:PRO:HD2	2.01	0.90
1:B:591:THR:HG22	1:B:593:LEU:N	1.88	0.89
1:B:262:PHE:HE1	5:B:835:HOH:O	1.55	0.89
1:A:591:THR:HG22	1:A:593:LEU:N	1.88	0.89
1:A:555:HIS:HD2	5:A:878:HOH:O	1.56	0.88
1:B:591:THR:HG23	1:B:592:PRO:CD	2.05	0.87
1:A:141:ALA:HB2	1:A:278:VAL:HG21	1.56	0.87
1:A:323:GLY:O	1:A:491:ARG:HD2	1.75	0.87
1:A:461:THR:HG22	1:A:461:THR:O	1.72	0.86
1:B:574:LEU:HD12	5:B:875:HOH:O	1.75	0.86
1:A:270:MET:HE3	1:A:281:ILE:HD13	1.56	0.86
1:A:143:LEU:CD2	1:A:270:MET:HG2	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:CYS:HB3	5:B:98:HOH:O	1.76	0.85
1:B:175:GLN:O	1:B:210:ARG:NH1	2.11	0.84
1:A:471:THR:CG2	5:A:851:HOH:O	2.24	0.84
1:B:381:ASP:HB3	5:B:841:HOH:O	1.77	0.84
1:B:141:ALA:HB2	1:B:278:VAL:HG21	1.57	0.84
1:B:672:GLN:HG2	1:B:674:PHE:CZ	2.12	0.83
1:B:270:MET:HE3	1:B:281:ILE:HD13	1.61	0.83
1:B:143:LEU:CD2	1:B:270:MET:HG2	2.07	0.83
1:A:674:PHE:HE2	1:A:722:ILE:HD13	1.44	0.83
1:A:669:LEU:HD13	1:A:669:LEU:C	2.04	0.82
1:B:447:LYS:CE	5:B:829:HOH:O	2.27	0.82
1:A:352:ASN:HD22	1:A:352:ASN:C	1.86	0.81
1:A:352:ASN:ND2	1:A:354:LEU:H	1.78	0.81
1:A:579:LYS:HB3	1:A:580:PRO:HD2	1.60	0.81
1:A:727:ASP:OD1	1:A:731:SER:HB3	1.81	0.81
1:A:144:ASP:HB3	1:A:146:GLY:N	1.94	0.80
1:B:352:ASN:C	1:B:352:ASN:HD22	1.90	0.80
1:B:323:GLY:O	1:B:491:ARG:HD2	1.81	0.80
1:B:523:THR:HG23	5:B:945:HOH:O	1.81	0.79
1:B:674:PHE:HE2	1:B:722:ILE:HD13	1.46	0.79
2:C:1:NAG:O6	2:C:2:NAG:C1	2.30	0.79
1:A:731:SER:HA	5:A:785:HOH:O	1.83	0.79
1:B:579:LYS:HB3	1:B:580:PRO:HD2	1.63	0.79
1:B:238:PRO:HD2	5:B:106:HOH:O	1.81	0.79
1:B:128:LEU:HD13	1:B:550:MET:HE3	1.64	0.78
1:B:352:ASN:ND2	1:B:354:LEU:H	1.79	0.78
1:A:128:LEU:HD13	1:A:550:MET:HE3	1.66	0.78
1:B:450:LYS:HG2	5:B:912:HOH:O	1.83	0.78
1:B:446:LYS:HD3	5:B:901:HOH:O	1.83	0.78
1:B:669:LEU:C	1:B:669:LEU:HD13	2.09	0.78
1:B:447:LYS:HE3	5:B:829:HOH:O	1.84	0.78
1:A:471:THR:HG22	5:A:851:HOH:O	1.83	0.77
1:B:388:LEU:O	1:B:391:VAL:HG12	1.85	0.77
1:A:591:THR:CG2	1:A:592:PRO:CD	2.61	0.76
1:A:388:LEU:O	1:A:391:VAL:HG12	1.84	0.76
1:A:346:GLY:HA2	1:A:467:THR:O	1.85	0.76
1:B:591:THR:CG2	1:B:592:PRO:CD	2.63	0.76
1:B:346:GLY:HA2	1:B:467:THR:O	1.86	0.76
1:B:727:ASP:OD1	1:B:731:SER:HB3	1.85	0.76
1:B:116:THR:HG21	1:B:543:HIS:NE2	2.01	0.76
1:B:663:ILE:H	1:B:663:ILE:HD13	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:ILE:HD13	1:A:663:ILE:H	1.50	0.75
1:B:493:TYR:CE1	5:B:845:HOH:O	2.39	0.75
1:A:552:LYS:CD	5:A:837:HOH:O	2.34	0.75
1:B:634:LYS:O	1:B:638:ARG:HA	1.85	0.74
3:G:1:NAG:C4	3:G:3:NAG:C1	2.66	0.74
1:A:116:THR:HG21	1:A:543:HIS:NE2	2.03	0.74
1:A:365:ARG:NE	5:A:913:HOH:O	2.20	0.73
3:G:1:NAG:O4	3:G:3:NAG:O5	2.07	0.73
1:B:381:ASP:CB	5:B:841:HOH:O	2.35	0.72
1:A:460:VAL:O	1:A:461:THR:HB	1.89	0.72
1:A:552:LYS:HD2	5:A:837:HOH:O	1.90	0.72
1:A:123:ASN:HD22	1:A:125:SER:H	1.38	0.72
1:A:393:ASN:O	1:A:397:THR:CG2	2.37	0.71
1:B:586:ASN:HD22	1:B:587:ASN:N	1.88	0.71
1:A:176:PHE:HA	1:A:180:MET:HE3	1.72	0.71
1:B:393:ASN:O	1:B:397:THR:CG2	2.37	0.71
1:B:460:VAL:O	1:B:461:THR:HB	1.90	0.71
1:A:472:TYR:HB3	5:A:782:HOH:O	1.91	0.71
1:A:577:THR:O	1:A:578:ARG:HB2	1.91	0.71
1:A:302:PHE:O	1:A:306:MET:HG2	1.92	0.70
1:A:575:ASP:OD1	1:A:575:ASP:C	2.34	0.70
1:B:176:PHE:HA	1:B:180:MET:HE3	1.75	0.69
1:A:586:ASN:HD22	1:A:587:ASN:N	1.91	0.69
1:B:450:LYS:CG	5:B:912:HOH:O	2.41	0.69
1:B:375:TYR:CD2	5:B:821:HOH:O	2.24	0.69
1:B:384:SER:O	1:B:388:LEU:HD23	1.93	0.69
1:A:384:SER:O	1:A:388:LEU:HD23	1.93	0.68
5:A:829:HOH:O	3:E:1:NAG:H83	1.93	0.68
1:A:578:ARG:HE	1:A:578:ARG:HA	1.59	0.68
1:A:470:GLU:HA	5:A:10:HOH:O	1.93	0.68
1:B:218:HIS:CE1	1:B:510:ALA:HB3	2.29	0.68
3:G:1:NAG:C6	3:G:3:NAG:C1	2.72	0.68
1:A:570:THR:HG21	1:A:605:ALA:HB2	1.75	0.68
1:B:674:PHE:CE2	1:B:722:ILE:HD13	2.24	0.68
1:A:591:THR:HG22	1:A:592:PRO:N	2.09	0.67
1:A:352:ASN:C	1:A:352:ASN:ND2	2.52	0.67
1:A:578:ARG:HA	1:A:578:ARG:NE	2.09	0.67
1:A:129:TRP:CG	1:A:134:LEU:HD22	2.30	0.67
1:A:702:VAL:HG22	1:A:703:SER:N	2.10	0.67
1:B:123:ASN:HD21	1:B:126:SER:H	1.42	0.67
1:B:570:THR:HG21	1:B:605:ALA:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:THR:HG22	1:B:592:PRO:N	2.09	0.67
1:B:177:ASN:H	1:B:180:MET:CE	2.06	0.67
1:B:721:THR:CG2	5:B:784:HOH:O	2.29	0.67
1:B:129:TRP:CG	1:B:134:LEU:HD22	2.30	0.67
1:B:302:PHE:O	1:B:306:MET:HG2	1.94	0.67
1:A:199:ASP:OD1	1:A:201:THR:HB	1.94	0.66
1:B:199:ASP:OD1	1:B:201:THR:HB	1.95	0.66
1:A:634:LYS:O	1:A:638:ARG:HA	1.95	0.66
1:B:123:ASN:HD22	1:B:125:SER:H	1.41	0.66
1:B:433:ARG:NH2	5:B:101:HOH:O	2.28	0.66
3:G:2:FUC:C6	3:G:3:NAG:H2	2.26	0.66
1:A:460:VAL:HG22	5:A:863:HOH:O	1.96	0.66
1:B:702:VAL:HG22	1:B:703:SER:N	2.11	0.66
1:B:491:ARG:HG3	5:B:976:HOH:O	1.96	0.65
1:A:502:LEU:O	1:A:600:VAL:HG23	1.96	0.65
1:A:218:HIS:CE1	1:A:510:ALA:HB3	2.31	0.65
1:B:128:LEU:HD22	1:B:550:MET:HB3	1.78	0.65
1:B:237:ALA:H	1:B:471:THR:HG21	1.60	0.65
1:A:591:THR:CG2	1:A:592:PRO:N	2.60	0.65
1:A:237:ALA:H	1:A:471:THR:HG21	1.60	0.65
1:A:428:ASP:OD1	1:A:428:ASP:C	2.39	0.65
1:A:177:ASN:HD22	2:C:1:NAG:C1	2.01	0.64
1:A:411:MET:HE1	1:A:437:PHE:CE1	2.32	0.64
1:B:502:LEU:O	1:B:600:VAL:HG23	1.98	0.64
1:A:674:PHE:CD2	1:A:722:ILE:HD11	2.31	0.64
1:B:461:THR:O	1:B:461:THR:CG2	2.44	0.64
1:A:476:LYS:NZ	5:A:800:HOH:O	2.31	0.64
1:A:123:ASN:HD21	1:A:126:SER:H	1.45	0.63
1:A:136:GLN:HA	1:A:247:ARG:O	1.98	0.63
1:B:674:PHE:CD2	1:B:722:ILE:HD11	2.31	0.63
1:A:177:ASN:H	1:A:180:MET:CE	2.11	0.62
3:G:3:NAG:C1	3:G:3:NAG:O7	2.47	0.62
1:B:136:GLN:HA	1:B:247:ARG:O	1.99	0.62
1:B:591:THR:CG2	1:B:592:PRO:N	2.63	0.62
1:B:583:ASP:HB3	1:B:586:ASN:HD21	1.64	0.62
1:A:583:ASP:HB3	1:A:586:ASN:HD21	1.65	0.62
1:B:375:TYR:OH	1:B:377:LYS:HE3	2.00	0.61
1:B:700:ILE:HG22	1:B:722:ILE:HG23	1.82	0.61
1:A:270:MET:HE3	1:A:281:ILE:CD1	2.30	0.61
1:A:524:ASN:HD22	1:A:524:ASN:H	1.48	0.61
1:A:129:TRP:HB3	1:A:134:LEU:CD2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:TYR:OH	1:A:377:LYS:HE3	2.01	0.61
1:A:669:LEU:C	1:A:669:LEU:CD1	2.74	0.61
1:B:411:MET:HE1	1:B:437:PHE:CE1	2.35	0.61
1:A:591:THR:CG2	1:A:593:LEU:H	1.97	0.60
1:B:121:LYS:HD3	5:B:780:HOH:O	2.01	0.60
1:B:181:CYS:CB	5:B:98:HOH:O	2.39	0.60
1:B:689:LYS:HD2	1:B:742:GLN:OE1	2.00	0.60
1:A:701:SER:OG	1:A:721:THR:HG23	2.00	0.60
1:B:129:TRP:HB3	1:B:134:LEU:CD2	2.31	0.60
1:B:622:LEU:C	1:B:622:LEU:CD2	2.74	0.60
1:A:674:PHE:CE2	1:A:722:ILE:HD13	2.23	0.60
1:A:700:ILE:HG22	1:A:722:ILE:HG23	1.82	0.60
1:B:175:GLN:NE2	5:B:897:HOH:O	2.35	0.60
1:B:270:MET:HE3	1:B:281:ILE:CD1	2.32	0.60
1:A:345:ALA:HB3	1:A:472:TYR:HE1	1.66	0.60
1:B:428:ASP:C	1:B:428:ASP:OD1	2.45	0.60
1:A:622:LEU:C	1:A:622:LEU:CD2	2.75	0.60
1:A:689:LYS:HD2	1:A:742:GLN:OE1	2.02	0.60
1:B:457:LYS:HE3	5:B:821:HOH:O	2.01	0.60
1:B:325:LEU:C	1:B:325:LEU:HD12	2.27	0.59
1:B:610:LEU:HB3	1:B:678:VAL:HG22	1.83	0.59
1:B:266:LEU:O	1:B:266:LEU:HD12	2.02	0.59
1:A:433:ARG:NH2	5:A:95:HOH:O	2.33	0.59
1:A:569:THR:HA	1:A:749:ARG:O	2.01	0.59
1:A:325:LEU:C	1:A:325:LEU:HD12	2.28	0.59
1:A:610:LEU:HB3	1:A:678:VAL:HG22	1.84	0.59
1:A:199:ASP:CG	5:A:872:HOH:O	2.45	0.59
1:B:461:THR:N	1:B:462:PRO:CD	2.65	0.59
1:A:622:LEU:O	1:A:626:LEU:HD13	2.03	0.59
1:B:138:VAL:HG11	1:B:549:ALA:HB1	1.84	0.59
1:B:679:THR:HB	1:B:715:LYS:HG2	1.85	0.59
1:B:737:ILE:HD11	1:B:739:TRP:CZ3	2.37	0.59
4:F:1:NAG:H3	4:F:2:FUC:H5	1.85	0.59
1:B:524:ASN:H	1:B:524:ASN:HD22	1.49	0.58
1:B:566:ALA:O	1:B:570:THR:HG22	2.03	0.58
1:A:138:VAL:HG11	1:A:549:ALA:HB1	1.85	0.58
3:G:1:NAG:C4	3:G:3:NAG:O5	2.50	0.58
1:B:722:ILE:H	1:B:722:ILE:HD12	1.69	0.58
1:B:737:ILE:CD1	1:B:739:TRP:CZ3	2.86	0.58
1:B:388:LEU:O	1:B:391:VAL:CG1	2.52	0.58
3:G:1:NAG:HO4	3:G:3:NAG:C1	2.13	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:THR:HB	1:A:715:LYS:HG2	1.83	0.58
1:A:737:ILE:HD11	1:A:739:TRP:CZ3	2.39	0.58
1:B:345:ALA:HB3	1:B:472:TYR:HE1	1.68	0.58
1:B:701:SER:OG	1:B:721:THR:HG23	2.04	0.58
1:A:461:THR:N	1:A:462:PRO:CD	2.67	0.58
1:A:630:GLU:HB3	1:A:643:HIS:CD2	2.38	0.58
1:A:737:ILE:CD1	1:A:739:TRP:CZ3	2.87	0.58
1:A:357:ARG:HH12	1:A:474:ASP:CG	2.11	0.58
1:B:218:HIS:HD2	1:B:539:MET:HE2	1.68	0.58
1:B:518:ALA:CB	1:B:529:THR:HG22	2.34	0.58
1:A:352:ASN:HD22	1:A:354:LEU:H	1.49	0.57
1:A:388:LEU:O	1:A:391:VAL:CG1	2.52	0.57
1:A:385:GLU:HG2	1:A:413:ILE:HD12	1.85	0.57
5:A:829:HOH:O	3:E:1:NAG:C8	2.51	0.57
1:A:564:ARG:O	1:A:568:MET:HG3	2.04	0.57
1:A:672:GLN:CG	1:A:674:PHE:CZ	2.86	0.57
1:B:570:THR:HG21	1:B:605:ALA:CB	2.35	0.57
1:A:722:ILE:HD12	1:A:722:ILE:H	1.69	0.57
1:A:428:ASP:OD1	1:A:430:GLY:N	2.33	0.57
1:A:570:THR:HG21	1:A:605:ALA:CB	2.35	0.57
1:B:591:THR:CG2	1:B:593:LEU:H	1.97	0.57
1:B:352:ASN:C	1:B:352:ASN:ND2	2.55	0.57
1:B:290:ILE:HD13	1:B:290:ILE:H	1.69	0.56
1:B:123:ASN:ND2	1:B:126:SER:H	2.02	0.56
1:A:128:LEU:HD22	1:A:550:MET:HB3	1.85	0.56
1:A:229:LYS:CG	5:A:94:HOH:O	2.53	0.56
1:A:666:ASN:ND2	5:A:884:HOH:O	2.37	0.56
1:B:325:LEU:HA	1:B:486:ALA:HB1	1.88	0.56
1:B:669:LEU:C	1:B:669:LEU:CD1	2.78	0.56
1:A:176:PHE:CE2	1:A:180:MET:HB3	2.41	0.56
1:A:702:VAL:HG22	1:A:703:SER:H	1.70	0.56
1:B:732:ARG:HD3	1:B:732:ARG:N	2.20	0.56
1:A:150:GLU:OE2	1:A:210:ARG:NH2	2.39	0.56
1:A:586:ASN:ND2	1:A:588:LYS:H	2.04	0.56
1:B:266:LEU:HD12	1:B:266:LEU:C	2.30	0.56
1:B:352:ASN:HD22	1:B:354:LEU:H	1.51	0.56
1:B:574:LEU:CD1	5:B:875:HOH:O	2.42	0.56
1:A:722:ILE:HD12	1:A:722:ILE:N	2.21	0.56
1:B:630:GLU:HB3	1:B:643:HIS:CD2	2.41	0.56
3:G:2:FUC:H62	3:G:3:NAG:H2	1.88	0.56
1:A:566:ALA:O	1:A:570:THR:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:THR:HA	1:B:749:ARG:O	2.06	0.56
1:A:266:LEU:C	1:A:266:LEU:HD12	2.31	0.56
1:B:486:ALA:HB2	5:B:796:HOH:O	2.05	0.56
1:A:493:TYR:CE2	1:A:495:GLY:HA3	2.40	0.55
1:A:737:ILE:HD11	1:A:739:TRP:CH2	2.41	0.55
1:B:201:THR:O	1:B:201:THR:CG2	2.55	0.55
1:A:266:LEU:HD12	1:A:266:LEU:O	2.06	0.55
1:A:123:ASN:HD22	1:A:125:SER:N	2.04	0.55
1:A:461:THR:O	1:A:461:THR:CG2	2.46	0.55
3:E:2:FUC:H5	3:E:3:NAG:O5	2.06	0.55
1:A:352:ASN:HD22	1:A:353:GLY:N	2.04	0.55
1:B:722:ILE:HD12	1:B:722:ILE:N	2.22	0.55
1:B:570:THR:HG21	1:B:605:ALA:CA	2.37	0.55
1:B:622:LEU:O	1:B:626:LEU:HD13	2.06	0.55
1:A:201:THR:CG2	1:A:201:THR:O	2.54	0.55
1:A:570:THR:HG21	1:A:605:ALA:CA	2.36	0.55
1:B:385:GLU:HG2	1:B:413:ILE:HD12	1.88	0.55
1:B:570:THR:OG1	1:B:604:ARG:HB3	2.07	0.55
1:A:518:ALA:CB	1:A:529:THR:HG22	2.36	0.55
1:B:737:ILE:HD11	1:B:739:TRP:CH2	2.41	0.55
1:A:144:ASP:OD1	1:A:216:GLY:HA2	2.07	0.55
1:A:290:ILE:HD13	1:A:290:ILE:H	1.72	0.55
1:B:123:ASN:HD22	1:B:125:SER:N	2.04	0.54
1:A:760:VAL:CG1	1:A:761:TRP:N	2.70	0.54
1:A:325:LEU:HA	1:A:486:ALA:HB1	1.89	0.54
1:A:390:GLN:HE22	3:E:3:NAG:HN2	1.54	0.54
1:B:637:ALA:O	1:B:640:SER:OG	2.26	0.54
1:A:579:LYS:HB2	5:A:950:HOH:O	2.07	0.54
1:A:460:VAL:CG2	5:A:863:HOH:O	2.54	0.54
1:B:760:VAL:CG1	1:B:761:TRP:N	2.70	0.54
1:B:179:SER:HB3	4:F:1:NAG:H82	1.89	0.54
1:A:570:THR:OG1	1:A:604:ARG:HB3	2.06	0.53
1:A:669:LEU:HD13	1:A:670:LEU:N	2.23	0.53
1:B:697:ASN:ND2	5:B:970:HOH:O	2.41	0.53
1:B:586:ASN:ND2	1:B:588:LYS:H	2.07	0.53
1:B:679:THR:HG22	5:B:790:HOH:O	2.09	0.53
1:B:760:VAL:HG12	1:B:761:TRP:N	2.23	0.53
1:A:233:HIS:O	1:A:233:HIS:CD2	2.62	0.53
1:B:541:ALA:N	1:B:542:PRO:HD2	2.24	0.53
1:A:390:GLN:NE2	3:E:1:NAG:O6	2.42	0.53
1:A:661:TYR:CD2	1:A:726:GLY:HA3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:TYR:CB	1:A:739:TRP:HD1	2.22	0.53
1:A:760:VAL:HG12	1:A:761:TRP:N	2.24	0.53
1:B:564:ARG:O	1:B:568:MET:HG3	2.09	0.53
1:B:658:ILE:HG22	5:B:782:HOH:O	2.08	0.53
1:A:288:ARG:HG3	1:A:326:ASN:HB3	1.91	0.53
1:A:610:LEU:HB2	1:A:748:VAL:HG21	1.90	0.53
1:A:123:ASN:ND2	1:A:126:SER:H	2.05	0.53
1:A:697:ASN:CG	5:A:857:HOH:O	2.51	0.53
1:A:749:ARG:HB3	5:A:844:HOH:O	2.08	0.53
1:B:352:ASN:HD22	1:B:353:GLY:N	2.07	0.53
1:A:732:ARG:HD3	1:A:732:ARG:N	2.23	0.52
1:B:218:HIS:ND1	1:B:510:ALA:HB3	2.24	0.52
1:B:392:GLU:N	5:B:921:HOH:O	2.42	0.52
1:A:120:LEU:O	1:A:121:LYS:HB2	2.09	0.52
1:A:427:GLU:OE2	1:A:445:ASN:HB2	2.09	0.52
3:G:1:NAG:H4	3:G:3:NAG:O5	2.09	0.52
1:B:610:LEU:HB2	1:B:748:VAL:HG21	1.92	0.52
1:B:666:ASN:HB2	5:B:899:HOH:O	2.07	0.52
1:A:218:HIS:HD2	1:A:539:MET:HE2	1.73	0.52
1:A:634:LYS:HB3	1:A:634:LYS:HZ3	1.75	0.52
1:A:541:ALA:N	1:A:542:PRO:HD2	2.25	0.52
1:A:169:ILE:HG12	5:A:952:HOH:O	2.08	0.52
1:A:418:ARG:HG3	1:B:418:ARG:NH2	2.25	0.52
1:B:326:ASN:C	1:B:326:ASN:HD22	2.18	0.52
1:A:566:ALA:O	1:A:570:THR:CG2	2.58	0.52
1:B:702:VAL:HG22	1:B:703:SER:H	1.73	0.52
1:B:718:TYR:CZ	1:B:739:TRP:CZ3	2.98	0.52
1:B:199:ASP:OD1	1:B:199:ASP:C	2.54	0.51
1:B:688:TYR:CB	1:B:739:TRP:HD1	2.23	0.51
1:A:263:THR:HG23	1:A:296:ALA:HB2	1.92	0.51
1:A:345:ALA:CB	1:A:472:TYR:HE1	2.22	0.51
1:A:342:ARG:HD3	1:A:344:PHE:CE2	2.46	0.51
1:B:120:LEU:O	1:B:121:LYS:HB2	2.09	0.51
1:B:491:ARG:HH21	1:B:759:GLU:HB2	1.75	0.51
1:A:718:TYR:CZ	1:A:739:TRP:CZ3	2.98	0.51
1:B:566:ALA:O	1:B:570:THR:CG2	2.58	0.51
1:B:610:LEU:HB3	1:B:678:VAL:CG2	2.40	0.51
1:B:688:TYR:HB3	1:B:739:TRP:HD1	1.76	0.51
1:B:669:LEU:HD13	1:B:670:LEU:N	2.26	0.51
1:B:288:ARG:HG3	1:B:326:ASN:HB3	1.92	0.50
1:A:540:ALA:O	1:A:543:HIS:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:LEU:HB3	1:A:678:VAL:CG2	2.40	0.50
1:A:352:ASN:HD21	1:A:354:LEU:CB	2.24	0.50
1:B:342:ARG:HD3	1:B:344:PHE:CE2	2.46	0.50
1:A:157:ASP:CG	5:A:909:HOH:O	2.54	0.50
1:B:176:PHE:CE2	1:B:180:MET:HB3	2.47	0.50
1:B:366:ALA:HB3	1:B:468:PHE:CE1	2.46	0.50
1:B:368:VAL:HG22	1:B:368:VAL:O	2.12	0.50
1:B:427:GLU:OE2	1:B:445:ASN:HB2	2.11	0.50
1:B:661:TYR:CD2	1:B:726:GLY:HA3	2.47	0.50
1:A:562:ALA:O	1:A:565:SER:HB3	2.12	0.50
1:A:577:THR:O	1:A:578:ARG:CB	2.58	0.49
1:B:622:LEU:O	1:B:622:LEU:HD23	2.11	0.49
1:A:368:VAL:O	1:A:368:VAL:HG22	2.12	0.49
1:A:622:LEU:O	1:A:622:LEU:HD23	2.10	0.49
1:B:586:ASN:O	1:B:587:ASN:HB2	2.12	0.49
1:B:663:ILE:HD13	1:B:663:ILE:N	2.23	0.49
1:A:143:LEU:CD2	1:A:270:MET:CG	2.86	0.49
1:B:731:SER:N	5:B:960:HOH:O	2.44	0.49
3:D:1:NAG:H61	3:D:3:NAG:O7	2.13	0.49
3:G:2:FUC:H61	3:G:3:NAG:H2	1.95	0.49
1:A:346:GLY:O	1:A:442:VAL:HG11	2.13	0.49
1:A:512:TYR:HE1	5:A:773:HOH:O	1.93	0.49
1:A:418:ARG:NH2	1:B:418:ARG:HG3	2.28	0.49
1:B:147:ILE:N	1:B:211:ASP:HB2	2.28	0.49
1:B:433:ARG:HD2	5:B:51:HOH:O	2.11	0.49
1:B:448:GLU:HA	1:B:451:GLN:HE21	1.78	0.49
1:A:326:ASN:C	1:A:326:ASN:HD22	2.21	0.49
1:B:128:LEU:CD2	1:B:550:MET:HB3	2.42	0.49
1:A:357:ARG:NH1	1:A:474:ASP:OD2	2.40	0.49
1:B:218:HIS:CD2	1:B:539:MET:HE2	2.48	0.49
1:B:562:ALA:O	1:B:565:SER:HB3	2.12	0.49
1:A:166:TRP:CZ2	1:A:168:GLY:HA3	2.48	0.49
1:B:129:TRP:CB	1:B:134:LEU:CD2	2.90	0.48
1:B:407:PHE:CD2	1:B:431:VAL:HG22	2.48	0.48
1:B:628:PHE:HB3	1:B:632:GLN:HB2	1.96	0.48
1:A:129:TRP:CB	1:A:134:LEU:CD2	2.91	0.48
1:A:575:ASP:OD1	1:A:577:THR:N	2.34	0.48
1:B:233:HIS:O	1:B:233:HIS:CD2	2.67	0.48
1:B:372:PRO:HD2	1:B:396:ASN:O	2.13	0.48
1:B:263:THR:HG23	1:B:296:ALA:HB2	1.95	0.48
1:A:688:TYR:HB3	1:A:739:TRP:HD1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:LYS:HE2	5:B:829:HOH:O	2.03	0.48
1:B:166:TRP:CZ2	1:B:168:GLY:HA3	2.49	0.48
3:E:1:NAG:H61	3:E:3:NAG:C7	2.44	0.48
1:A:703:SER:HA	1:A:704:PRO:C	2.38	0.48
1:A:163:PRO:O	5:A:910:HOH:O	2.20	0.48
1:A:617:GLN:CB	5:A:808:HOH:O	2.62	0.48
1:B:129:TRP:HB3	1:B:134:LEU:HD21	1.95	0.48
1:B:290:ILE:HD13	1:B:290:ILE:N	2.28	0.48
1:A:350:LEU:N	1:A:350:LEU:HD12	2.29	0.48
1:A:628:PHE:HB3	1:A:632:GLN:HB2	1.95	0.48
1:A:218:HIS:ND1	1:A:510:ALA:HB3	2.29	0.47
1:A:366:ALA:HB3	1:A:468:PHE:CE1	2.48	0.47
1:B:143:LEU:CD2	1:B:270:MET:CG	2.87	0.47
1:B:247:ARG:NE	5:B:62:HOH:O	2.43	0.47
1:B:685:ALA:HB2	1:B:710:LYS:O	2.14	0.47
1:A:290:ILE:HD13	1:A:290:ILE:N	2.29	0.47
1:A:622:LEU:CD2	1:A:622:LEU:O	2.62	0.47
1:B:570:THR:HG21	1:B:605:ALA:HA	1.96	0.47
1:B:672:GLN:CG	1:B:674:PHE:CZ	2.92	0.47
1:A:177:ASN:O	1:A:180:MET:HB2	2.13	0.47
1:A:208:SER:O	1:A:254:LYS:HD3	2.14	0.47
1:B:493:TYR:CZ	5:B:845:HOH:O	2.65	0.47
1:A:491:ARG:HH21	1:A:759:GLU:HB2	1.78	0.47
1:B:237:ALA:N	1:B:238:PRO:CD	2.78	0.47
1:A:702:VAL:CG2	1:A:703:SER:N	2.77	0.47
1:B:500:ASP:OD2	1:B:564:ARG:HD2	2.15	0.47
1:A:357:ARG:NH2	1:A:474:ASP:OD2	2.45	0.47
1:A:367:PHE:N	1:B:526:LEU:O	2.44	0.47
1:B:129:TRP:CG	1:B:134:LEU:CD2	2.98	0.47
1:B:586:ASN:HD22	1:B:587:ASN:H	1.58	0.47
3:G:1:NAG:O4	3:G:2:FUC:H5	2.14	0.47
1:B:622:LEU:CD2	1:B:622:LEU:O	2.63	0.47
1:B:703:SER:HA	1:B:704:PRO:C	2.40	0.47
1:A:491:ARG:O	1:A:760:VAL:HG13	2.15	0.47
1:B:186:ILE:HD13	1:B:249:ARG:HB3	1.97	0.47
1:B:352:ASN:HD21	1:B:354:LEU:CB	2.27	0.47
1:A:199:ASP:OD1	1:A:199:ASP:C	2.57	0.46
1:A:399:VAL:CG1	1:A:419:LEU:HD13	2.44	0.46
1:A:689:LYS:HD3	5:A:862:HOH:O	2.14	0.46
1:B:393:ASN:N	1:B:394:PRO:CD	2.77	0.46
1:A:393:ASN:N	1:A:394:PRO:CD	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:ASN:HD22	1:B:586:ASN:C	2.21	0.46
1:B:177:ASN:N	1:B:180:MET:HE2	2.14	0.46
1:A:218:HIS:HE1	1:A:532:ILE:O	1.98	0.46
1:A:129:TRP:HB3	1:A:134:LEU:HD21	1.96	0.46
1:A:500:ASP:OD2	1:A:564:ARG:HD2	2.14	0.46
1:A:615:THR:O	1:A:618:ASP:HB2	2.15	0.46
1:B:399:VAL:CG1	1:B:419:LEU:HD13	2.45	0.46
1:B:575:ASP:C	1:B:575:ASP:OD1	2.58	0.46
1:A:586:ASN:HD22	1:A:586:ASN:C	2.22	0.46
1:B:177:ASN:O	1:B:180:MET:HB2	2.16	0.46
1:B:238:PRO:CD	5:B:106:HOH:O	2.53	0.46
1:B:345:ALA:CB	1:B:472:TYR:HE1	2.28	0.46
1:A:154:PHE:HE1	1:A:217:THR:HG23	1.81	0.46
1:A:668:THR:O	1:A:669:LEU:C	2.58	0.46
1:B:678:VAL:HG13	1:B:678:VAL:O	2.15	0.46
1:B:385:GLU:HG3	5:B:80:HOH:O	2.16	0.46
1:B:493:TYR:HE2	1:B:496:ILE:HG13	1.81	0.46
1:A:325:LEU:HA	1:A:486:ALA:CB	2.46	0.46
1:B:540:ALA:O	1:B:543:HIS:HB2	2.16	0.46
1:A:218:HIS:CD2	1:A:539:MET:HE2	2.50	0.45
1:A:407:PHE:CD2	1:A:431:VAL:HG22	2.50	0.45
1:A:446:LYS:N	5:A:899:HOH:O	2.48	0.45
1:A:663:ILE:HD13	1:A:663:ILE:N	2.24	0.45
1:B:329:SER:HB2	1:B:332:ILE:HD12	1.97	0.45
1:B:491:ARG:O	1:B:760:VAL:HG13	2.16	0.45
1:B:493:TYR:CE2	1:B:495:GLY:HA3	2.50	0.45
1:A:586:ASN:HD22	1:A:587:ASN:H	1.63	0.45
1:A:229:LYS:CB	5:A:94:HOH:O	2.64	0.45
3:G:1:NAG:C6	3:G:3:NAG:O7	2.53	0.45
1:A:147:ILE:N	1:A:211:ASP:HB2	2.31	0.45
1:B:208:SER:O	1:B:254:LYS:HD3	2.16	0.45
1:B:685:ALA:N	5:B:988:HOH:O	2.50	0.45
1:A:578:ARG:HE	1:A:578:ARG:CA	2.29	0.45
1:B:310:LEU:O	5:B:102:HOH:O	2.21	0.45
1:B:350:LEU:HD12	1:B:350:LEU:N	2.31	0.45
1:B:668:THR:O	1:B:669:LEU:C	2.59	0.45
1:A:390:GLN:NE2	3:E:3:NAG:N2	2.63	0.45
1:A:570:THR:HG21	1:A:605:ALA:HA	1.97	0.45
1:A:327:ASN:HA	5:A:951:HOH:O	2.16	0.45
1:A:727:ASP:OD1	1:A:731:SER:CB	2.60	0.45
1:A:129:TRP:CG	1:A:134:LEU:CD2	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ASP:OD1	1:B:182:ASN:HB2	2.17	0.45
1:A:198:ASN:HB2	5:A:799:HOH:O	2.16	0.45
1:A:481:VAL:O	1:A:584:SER:HB3	2.17	0.45
1:B:127:GLY:HA3	1:B:603:ASN:OD1	2.16	0.44
1:B:689:LYS:HD2	1:B:742:GLN:NE2	2.29	0.44
1:A:237:ALA:N	1:A:238:PRO:CD	2.80	0.44
1:A:574:LEU:HD23	1:A:580:PRO:HA	1.98	0.44
1:B:218:HIS:HE1	1:B:532:ILE:O	2.01	0.44
1:A:271:ASP:OD2	1:A:638:ARG:NH2	2.50	0.44
1:A:372:PRO:HD2	1:A:396:ASN:O	2.17	0.44
1:A:617:GLN:HB2	5:A:808:HOH:O	2.16	0.44
1:A:676:ARG:NH2	5:A:50:HOH:O	2.46	0.44
1:B:254:LYS:HE2	1:B:257:PHE:CD2	2.53	0.44
1:B:404:ASN:OD1	1:B:404:ASN:C	2.61	0.44
1:B:622:LEU:C	1:B:622:LEU:HD22	2.41	0.44
1:B:702:VAL:CG2	1:B:703:SER:N	2.78	0.44
1:A:128:LEU:CD2	1:A:550:MET:HB3	2.48	0.44
1:A:314:SER:HB2	1:A:537:THR:HB	1.99	0.44
1:A:129:TRP:CD2	1:A:134:LEU:HD22	2.52	0.44
1:A:379:LEU:HD12	1:A:380:SER:N	2.33	0.44
1:A:448:GLU:HA	1:A:451:GLN:HE21	1.83	0.44
1:B:218:HIS:CG	1:B:510:ALA:HB3	2.53	0.44
1:A:244:VAL:CG1	1:A:546:GLY:HA3	2.48	0.44
1:A:586:ASN:O	1:A:587:ASN:HB2	2.17	0.44
1:A:143:LEU:HD12	1:A:253:TYR:HB2	1.98	0.44
1:A:236:TYR:CE1	1:A:469:GLN:HA	2.53	0.44
1:A:622:LEU:C	1:A:622:LEU:HD22	2.43	0.44
1:B:734:VAL:CG2	1:B:735:GLY:N	2.81	0.44
1:A:404:ASN:OD1	1:A:404:ASN:C	2.60	0.44
1:A:524:ASN:HD22	1:A:524:ASN:N	2.15	0.43
1:B:129:TRP:CD2	1:B:134:LEU:HD22	2.52	0.43
1:B:192:ASN:ND2	1:B:207:ASN:OD1	2.51	0.43
1:A:123:ASN:ND2	1:A:125:SER:HB2	2.33	0.43
1:B:325:LEU:HA	1:B:486:ALA:CB	2.47	0.43
1:B:379:LEU:HD12	1:B:380:SER:N	2.33	0.43
1:A:352:ASN:HD21	1:A:354:LEU:H	1.64	0.43
1:A:329:SER:HB2	1:A:332:ILE:HD12	1.99	0.43
1:B:574:LEU:HD23	1:B:580:PRO:HA	2.00	0.43
1:A:488:GLY:HA3	1:A:498:LYS:O	2.18	0.43
1:A:685:ALA:HB2	1:A:710:LYS:O	2.18	0.43
1:A:718:TYR:CZ	1:A:739:TRP:CH2	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:LYS:HE3	1:B:696:LYS:HB2	1.86	0.43
1:A:528:SER:O	5:A:880:HOH:O	2.21	0.43
1:A:692:LEU:HB3	1:A:700:ILE:HD11	2.00	0.43
1:B:271:ASP:OD2	1:B:638:ARG:NH2	2.52	0.43
1:B:379:LEU:HD12	1:B:379:LEU:C	2.44	0.43
1:A:555:HIS:CB	5:A:878:HOH:O	2.66	0.43
1:B:481:VAL:O	1:B:584:SER:HB3	2.19	0.43
1:B:578:ARG:HE	1:B:578:ARG:HA	1.84	0.43
1:B:711:ASN:O	1:B:712:LYS:C	2.62	0.43
4:F:1:NAG:H3	4:F:2:FUC:C5	2.48	0.43
1:A:186:ILE:HD13	1:A:249:ARG:HB3	2.00	0.43
1:A:201:THR:HG23	5:A:915:HOH:O	2.18	0.43
1:B:123:ASN:ND2	1:B:125:SER:HB2	2.34	0.43
1:B:154:PHE:HE1	1:B:217:THR:HG23	1.84	0.43
1:B:518:ALA:HB2	1:B:529:THR:HG22	2.01	0.43
1:B:403:ASP:C	1:B:403:ASP:OD1	2.62	0.43
1:B:634:LYS:HZ3	1:B:634:LYS:HB3	1.83	0.43
1:A:379:LEU:HD12	1:A:379:LEU:C	2.44	0.42
1:A:678:VAL:O	1:A:678:VAL:HG13	2.18	0.42
1:B:663:ILE:H	1:B:663:ILE:CD1	2.26	0.42
1:B:236:TYR:CE1	1:B:469:GLN:HA	2.54	0.42
1:A:263:THR:O	1:A:266:LEU:HB3	2.18	0.42
1:A:447:LYS:N	5:A:899:HOH:O	2.26	0.42
1:A:192:ASN:ND2	1:A:207:ASN:OD1	2.53	0.42
1:A:352:ASN:HD21	1:A:354:LEU:HB2	1.85	0.42
1:B:615:THR:O	1:B:618:ASP:HB2	2.19	0.42
1:B:346:GLY:O	1:B:442:VAL:HG11	2.19	0.42
1:B:347:THR:HG21	1:B:355:LYS:HE3	2.02	0.42
1:A:218:HIS:CG	1:A:510:ALA:HB3	2.54	0.42
1:B:342:ARG:HD3	1:B:344:PHE:CZ	2.54	0.42
1:B:661:TYR:CD2	1:B:661:TYR:O	2.73	0.42
1:A:254:LYS:HE2	1:A:257:PHE:CD2	2.55	0.42
1:A:424:PHE:HB2	1:A:443:VAL:HG22	2.02	0.42
1:A:113:THR:HA	1:A:116:THR:HB	2.02	0.42
1:A:493:TYR:HE2	1:A:496:ILE:HG13	1.85	0.42
1:A:342:ARG:HD3	1:A:344:PHE:CZ	2.54	0.42
1:A:376:ASN:OD1	1:A:376:ASN:C	2.63	0.42
1:A:661:TYR:CD2	1:A:661:TYR:O	2.72	0.42
1:B:176:PHE:HA	1:B:180:MET:CE	2.48	0.42
1:A:127:GLY:HA3	1:A:603:ASN:OD1	2.19	0.42
1:A:156:ASP:OD1	1:A:182:ASN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:GLN:NE2	3:E:3:NAG:HN2	2.17	0.42
1:A:442:VAL:HG22	1:A:466:ILE:HD13	2.01	0.42
1:A:734:VAL:CG2	1:A:735:GLY:N	2.82	0.42
1:B:446:LYS:HA	5:B:901:HOH:O	2.18	0.42
1:A:399:VAL:HG12	1:A:419:LEU:HD13	2.02	0.41
1:A:270:MET:HB3	1:A:270:MET:HE2	1.76	0.41
1:B:113:THR:HA	1:B:116:THR:HB	2.02	0.41
1:B:237:ALA:N	1:B:471:THR:HG21	2.32	0.41
1:B:718:TYR:CZ	1:B:739:TRP:CH2	3.07	0.41
1:B:390:GLN:HE22	3:H:3:NAG:HN2	1.69	0.41
1:B:442:VAL:HG22	1:B:466:ILE:HD13	2.02	0.41
1:B:460:VAL:O	1:B:461:THR:CB	2.60	0.41
1:A:159:MET:HE1	1:A:247:ARG:O	2.21	0.41
1:B:394:PRO:HA	1:B:397:THR:HG23	2.03	0.41
1:A:242:ARG:HD3	1:A:242:ARG:N	2.36	0.41
1:A:626:LEU:HD23	1:A:628:PHE:CE1	2.55	0.41
1:A:702:VAL:CG2	1:A:703:SER:H	2.32	0.41
1:A:262:PHE:CE2	5:A:799:HOH:O	2.57	0.41
1:A:622:LEU:C	1:A:622:LEU:HD23	2.46	0.41
1:A:379:LEU:C	1:A:381:ASP:N	2.79	0.41
1:A:416:ARG:HD2	5:A:938:HOH:O	2.20	0.41
1:A:689:LYS:HD2	1:A:742:GLN:NE2	2.29	0.41
1:B:622:LEU:C	1:B:622:LEU:HD23	2.45	0.41
1:B:737:ILE:HG23	1:B:737:ILE:O	2.21	0.41
1:A:586:ASN:ND2	1:A:586:ASN:C	2.79	0.41
1:B:244:VAL:CG1	1:B:546:GLY:HA3	2.50	0.41
1:B:330:PRO:HB3	1:B:496:ILE:HD12	2.03	0.41
1:B:582:LYS:HD2	1:B:587:ASN:O	2.21	0.41
1:B:626:LEU:HD23	1:B:628:PHE:CE1	2.56	0.41
1:B:691:LYS:C	1:B:692:LEU:HD12	2.46	0.41
1:A:385:GLU:CG	1:A:413:ILE:HD12	2.51	0.40
1:A:524:ASN:ND2	1:A:525:ILE:HG13	2.36	0.40
1:A:582:LYS:HD2	1:A:587:ASN:O	2.22	0.40
1:B:159:MET:HE1	1:B:247:ARG:O	2.21	0.40
1:A:474:ASP:OD1	1:A:474:ASP:C	2.63	0.40
1:B:237:ALA:N	1:B:238:PRO:HD3	2.37	0.40
1:A:362:PHE:CE2	1:A:366:ALA:HB2	2.56	0.40
1:A:371:SER:HA	1:A:372:PRO:HD3	1.91	0.40
1:A:691:LYS:C	1:A:692:LEU:HD12	2.47	0.40
1:B:488:GLY:HA3	1:B:498:LYS:O	2.22	0.40
1:A:250:LEU:HD23	1:A:250:LEU:HA	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ASN:HB2	5:A:829:HOH:O	2.20	0.40
1:A:737:ILE:O	1:A:737:ILE:HG23	2.20	0.40
1:B:191:PHE:HA	5:B:825:HOH:O	2.21	0.40
1:B:292:LEU:HG	5:B:913:HOH:O	2.21	0.40
1:B:428:ASP:HA	1:B:429:PRO:HD2	1.92	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:3:NAG:O3	5:A:820:HOH:O[6_555]	2.12	0.08

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	632/649 (97%)	597 (94%)	32 (5%)	3 (0%)	24	43
1	B	625/649 (96%)	589 (94%)	34 (5%)	2 (0%)	36	55
All	All	1257/1298 (97%)	1186 (94%)	66 (5%)	5 (0%)	30	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	638	ARG
1	B	653	ASN
1	A	380	SER
1	A	461	THR
1	B	461	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	528/533 (99%)	480 (91%)	48 (9%)	9	19
1	B	525/533 (98%)	477 (91%)	48 (9%)	9	19
All	All	1053/1066 (99%)	957 (91%)	96 (9%)	9	19

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	THR
1	A	128	LEU
1	A	138	VAL
1	A	140	VAL
1	A	143	LEU
1	A	150	GLU
1	A	164	LYS
1	A	184	LYS
1	A	185	LEU
1	A	201	THR
1	A	223	THR
1	A	242	ARG
1	A	263	THR
1	A	266	LEU
1	A	270	MET
1	A	278	VAL
1	A	290	ILE
1	A	326	ASN
1	A	352	ASN
1	A	368	VAL
1	A	391	VAL
1	A	395	GLU
1	A	397	THR
1	A	414	ILE
1	A	442	VAL
1	A	460	VAL
1	A	471	THR

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Mol	Chain	Res	Type
1	A	502	LEU
1	A	524	ASN
1	A	586	ASN
1	A	600	VAL
1	A	622	LEU
1	A	624	CYS
1	A	634	LYS
1	A	638	ARG
1	A	645	CYS
1	A	652	LEU
1	A	663	ILE
1	A	668	THR
1	A	669	LEU
1	A	679	THR
1	A	687	THR
1	A	693	LYS
1	A	721	THR
1	A	722	ILE
1	A	732	ARG
1	A	734	VAL
1	A	740	VAL
1	B	116	THR
1	B	128	LEU
1	B	138	VAL
1	B	140	VAL
1	B	143	LEU
1	B	150	GLU
1	B	164	LYS
1	B	184	LYS
1	B	185	LEU
1	B	201	THR
1	B	223	THR
1	B	242	ARG
1	B	263	THR
1	B	266	LEU
1	B	270	MET
1	B	278	VAL
1	B	290	ILE
1	B	326	ASN
1	B	352	ASN
1	B	368	VAL
1	B	391	VAL

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Mol	Chain	Res	Type
1	B	395	GLU
1	B	397	THR
1	B	414	ILE
1	B	442	VAL
1	B	460	VAL
1	B	471	THR
1	B	502	LEU
1	B	524	ASN
1	B	586	ASN
1	B	600	VAL
1	B	622	LEU
1	B	624	CYS
1	B	634	LYS
1	B	638	ARG
1	B	645	CYS
1	B	652	LEU
1	B	663	ILE
1	B	668	THR
1	B	669	LEU
1	B	679	THR
1	B	687	THR
1	B	693	LYS
1	B	721	THR
1	B	722	ILE
1	B	732	ARG
1	B	734	VAL
1	B	740	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	136	GLN
1	A	175	GLN
1	A	218	HIS
1	A	326	ASN
1	A	327	ASN
1	A	352	ASN
1	A	390	GLN
1	A	451	GLN
1	A	524	ASN
1	A	555	HIS

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Mol	Chain	Res	Type
1	A	586	ASN
1	A	587	ASN
1	A	643	HIS
1	A	716	GLN
1	B	123	ASN
1	B	136	GLN
1	B	175	GLN
1	B	218	HIS
1	B	326	ASN
1	B	352	ASN
1	B	390	GLN
1	B	451	GLN
1	B	524	ASN
1	B	555	HIS
1	B	586	ASN
1	B	643	HIS
1	B	713	ASN
1	B	716	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

16 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	1,2	14,14,15	1.11	1 (7%)	17,19,21	1.67	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	2	2	14,14,15	0.82	0	17,19,21	2.07	5 (29%)
3	NAG	D	1	1,3	14,14,15	0.58	0	17,19,21	1.00	1 (5%)
3	FUC	D	2	3	10,10,11	0.76	0	14,14,16	1.28	2 (14%)
3	NAG	D	3	3	14,14,15	0.54	0	17,19,21	1.29	2 (11%)
3	NAG	E	1	1,3	14,14,15	0.44	0	17,19,21	9.00	6 (35%)
3	FUC	E	2	3	10,10,11	0.70	0	14,14,16	0.56	0
3	NAG	E	3	3	14,14,15	0.55	0	17,19,21	0.56	0
4	NAG	F	1	1,4	14,14,15	0.44	0	17,19,21	0.86	0
4	FUC	F	2	4	10,10,11	0.59	0	14,14,16	0.87	0
3	NAG	G	1	1,3	14,14,15	0.54	0	17,19,21	0.61	0
3	FUC	G	2	3	10,10,11	0.71	0	14,14,16	0.58	0
3	NAG	G	3	3	14,14,15	0.56	0	17,19,21	0.61	0
3	NAG	H	1	1,3	14,14,15	0.51	0	17,19,21	2.12	3 (17%)
3	FUC	H	2	3	10,10,11	0.64	0	14,14,16	0.52	0
3	NAG	H	3	3	14,14,15	0.53	0	17,19,21	0.80	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	D	2	3	-	-	0/1/1/1
3	NAG	D	3	3	-	1/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	E	2	3	-	-	0/1/1/1
3	NAG	E	3	3	-	1/6/23/26	0/1/1/1
4	NAG	F	1	1,4	1/1/5/7	2/6/23/26	0/1/1/1
4	FUC	F	2	4	-	-	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	G	2	3	-	-	0/1/1/1
3	NAG	G	3	3	-	5/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	3/6/23/26	0/1/1/1
3	FUC	H	2	3	-	-	0/1/1/1
3	NAG	H	3	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	O5-C1	-2.22	1.40	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	O7-C7-C8	-19.25	87.78	122.05
3	E	1	NAG	C8-C7-N2	18.47	146.75	116.12
3	E	1	NAG	O5-C1-C2	-17.50	84.21	111.29
3	E	1	NAG	C1-O5-C5	13.55	130.35	112.19
3	E	1	NAG	C4-C3-C2	-9.86	96.57	111.02
3	E	1	NAG	O3-C3-C2	8.55	127.16	109.40
3	H	1	NAG	C1-O5-C5	6.11	120.37	112.19
3	H	1	NAG	C4-C3-C2	-5.18	103.43	111.02
2	C	2	NAG	C4-C3-C2	-4.47	104.46	111.02
2	C	1	NAG	C4-C3-C2	-4.12	104.98	111.02
2	C	2	NAG	O5-C1-C2	-4.00	105.10	111.29
2	C	2	NAG	C1-C2-N2	3.53	116.00	110.43
3	D	3	NAG	C4-C3-C2	-3.21	106.31	111.02
3	D	1	NAG	O5-C1-C2	-3.03	106.61	111.29
3	D	3	NAG	O5-C1-C2	-2.89	106.82	111.29
2	C	2	NAG	C1-O5-C5	2.67	115.76	112.19
3	D	2	FUC	C3-C4-C5	2.57	113.72	109.81
3	D	2	FUC	C1-C2-C3	2.53	113.33	109.64
2	C	1	NAG	C2-N2-C7	-2.43	119.64	122.90
2	C	1	NAG	O4-C4-C3	-2.36	104.81	110.38
3	H	3	NAG	C2-N2-C7	-2.34	119.76	122.90
2	C	2	NAG	C2-N2-C7	-2.33	119.77	122.90
2	C	1	NAG	C3-C4-C5	-2.24	106.17	110.23
2	C	1	NAG	O6-C6-C5	-2.17	103.96	111.33
3	H	1	NAG	O5-C5-C4	2.15	116.06	110.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	1	NAG	C1

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2

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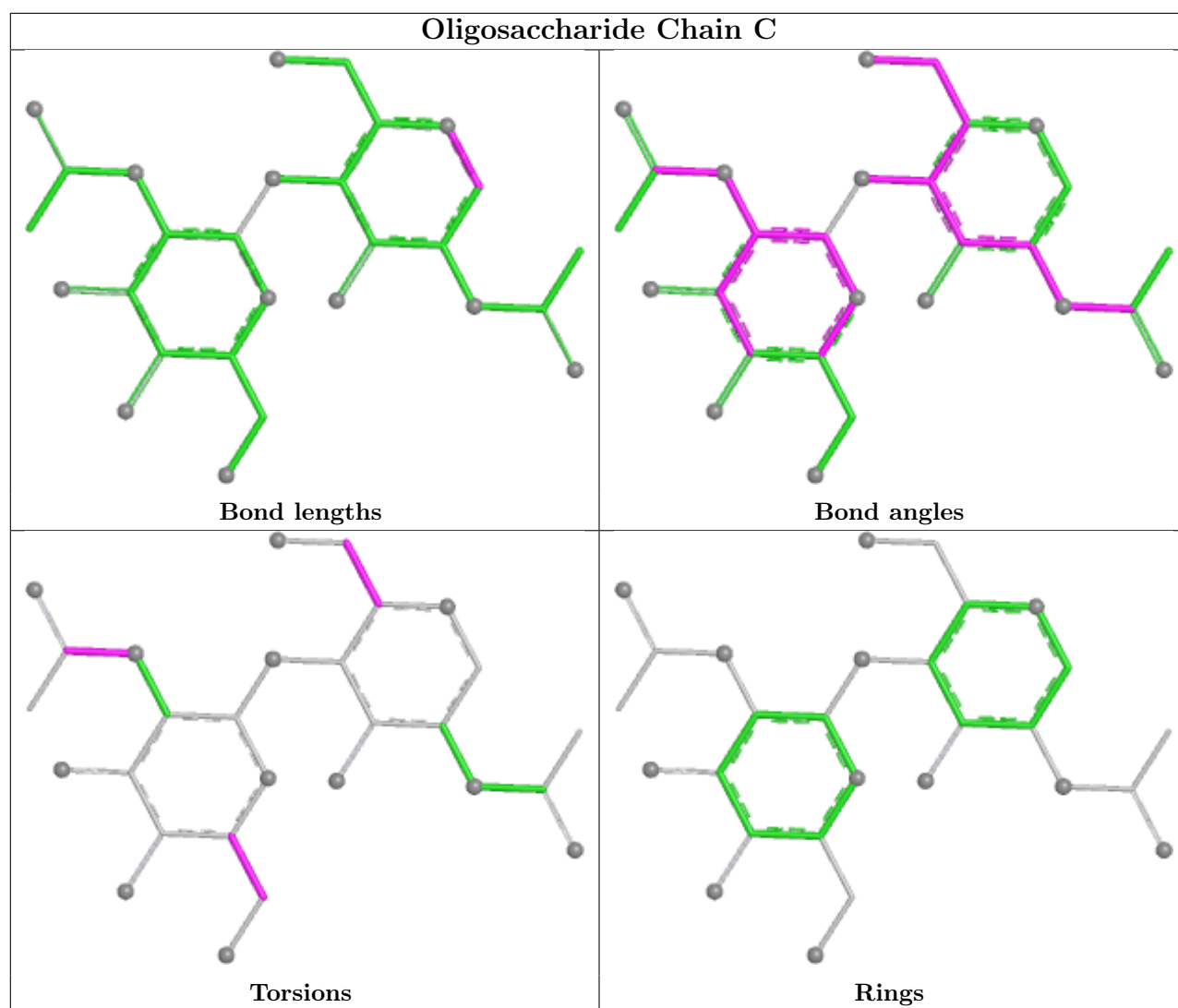
Mol	Chain	Res	Type	Atoms
3	D	3	NAG	C1-C2-N2-C7
3	E	1	NAG	C8-C7-N2-C2
3	G	3	NAG	C1-C2-N2-C7
3	H	1	NAG	C1-C2-N2-C7
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	G	3	NAG	C8-C7-N2-C2
4	F	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O7-C7-N2-C2
3	G	3	NAG	O7-C7-N2-C2
3	H	1	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
3	G	3	NAG	C4-C5-C6-O6
3	G	3	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C3-C2-N2-C7
3	E	3	NAG	O5-C5-C6-O6

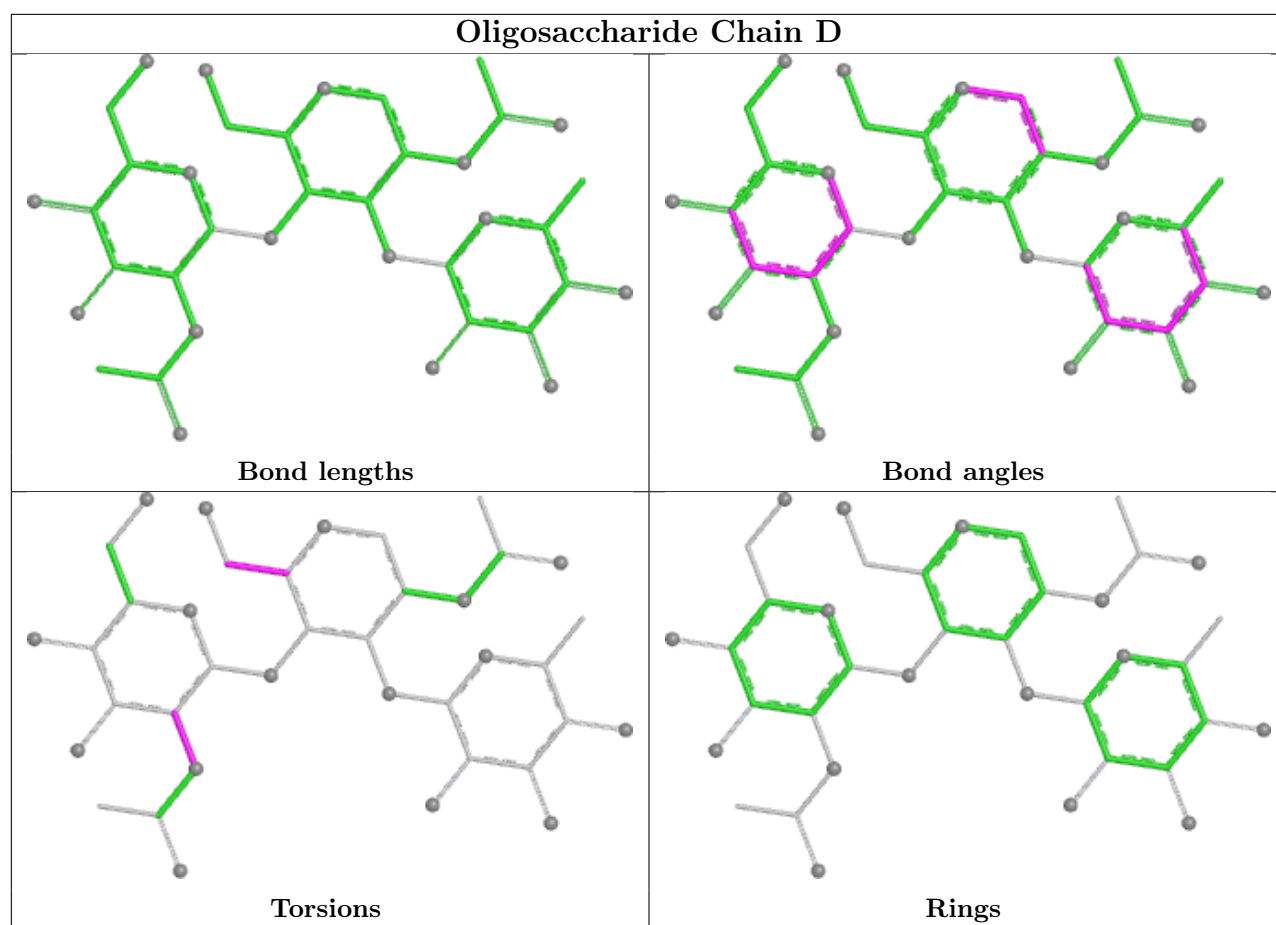
There are no ring outliers.

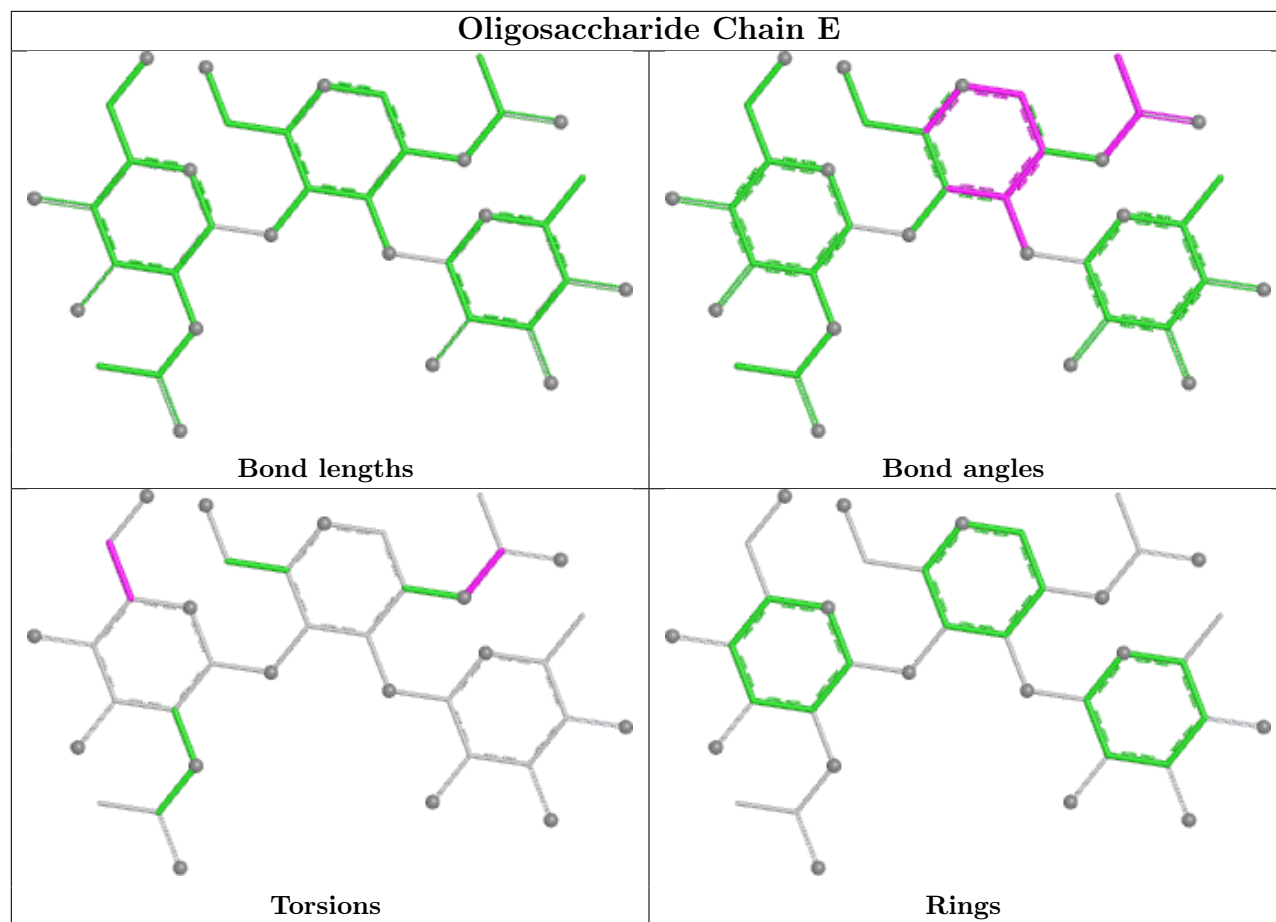
13 monomers are involved in 30 short contacts:

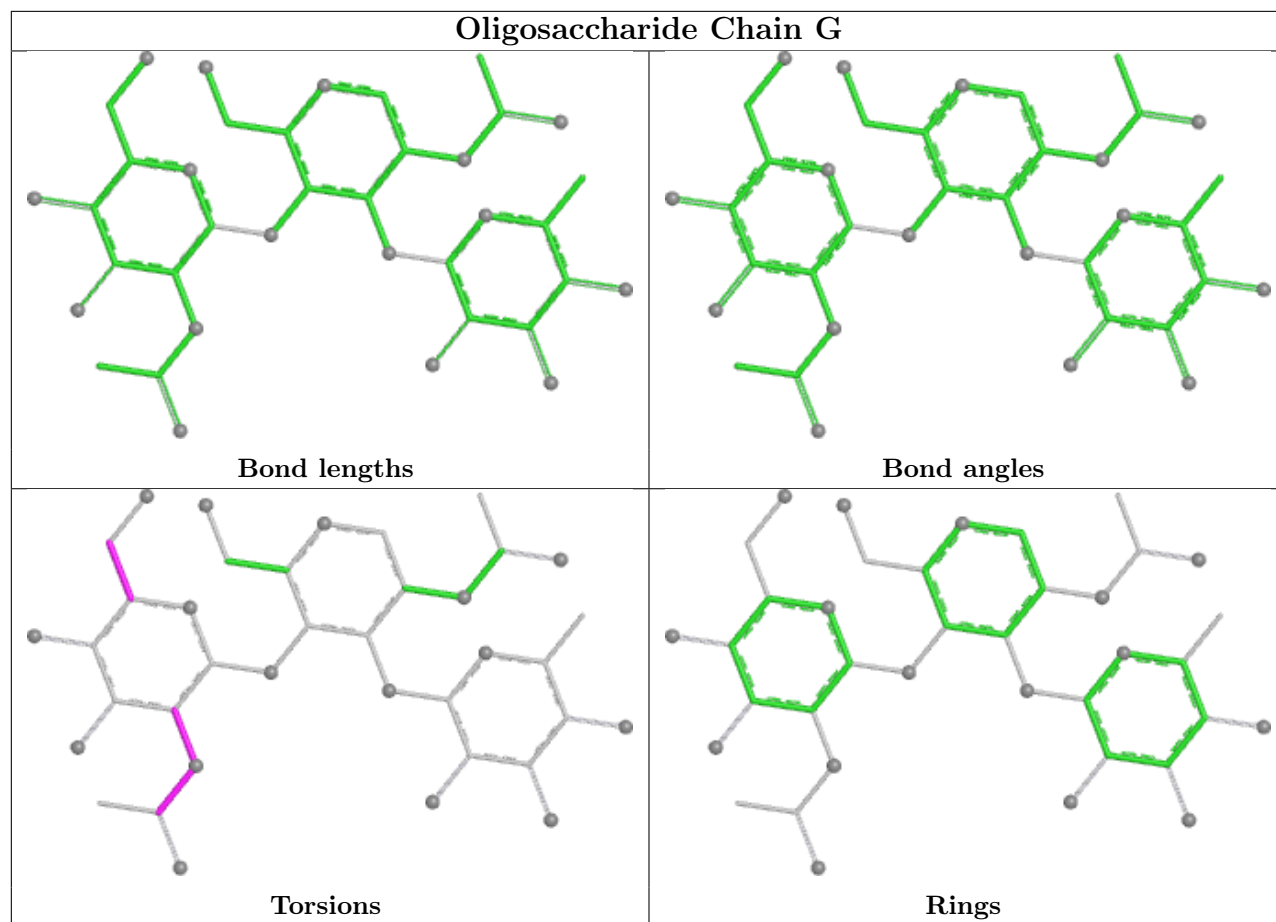
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3	NAG	1	0
3	H	3	NAG	1	0
4	F	1	NAG	3	0
3	G	3	NAG	13	1
2	C	1	NAG	2	0
3	G	2	FUC	4	0
2	C	2	NAG	1	0
3	G	1	NAG	10	0
3	E	1	NAG	4	0
4	F	2	FUC	2	0
3	E	3	NAG	5	0
3	E	2	FUC	1	0
3	D	1	NAG	1	0

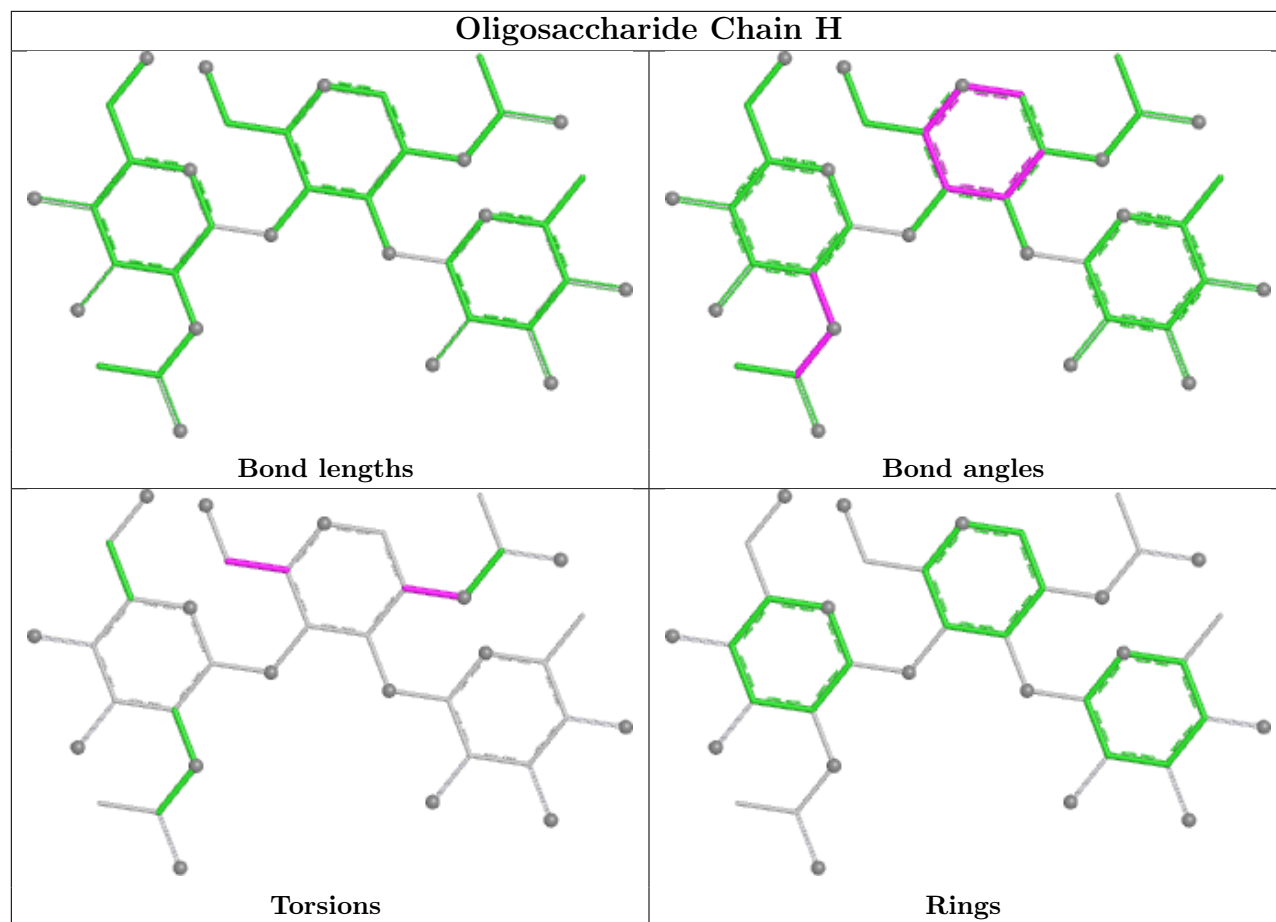
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

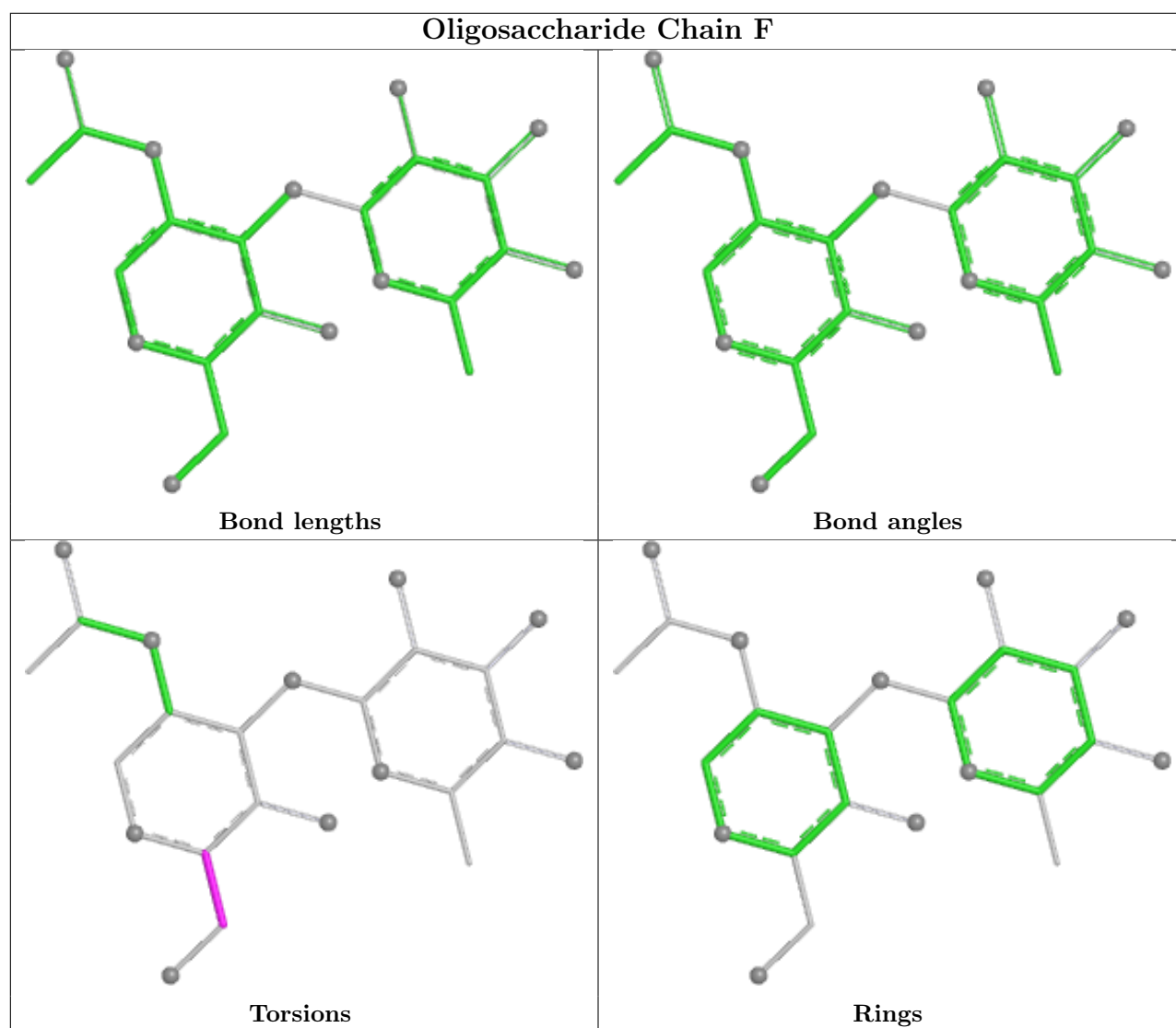












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	642/649 (98%)	0.40	18 (2%)	55 50	33, 48, 65, 79	0
1	B	639/649 (98%)	0.36	13 (2%)	65 61	33, 48, 65, 79	0
All	All	1281/1298 (98%)	0.38	31 (2%)	59 55	33, 48, 65, 79	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	667	PHE	4.3
1	A	645	CYS	4.1
1	A	144	ASP	3.8
1	A	739	TRP	3.6
1	B	739	TRP	3.5
1	A	590	ALA	3.2
1	B	722	ILE	3.1
1	A	725	ILE	3.0
1	B	645	CYS	2.9
1	B	705	GLN	2.7
1	B	386	GLU	2.6
1	B	380	SER	2.6
1	A	665	GLY	2.6
1	A	709	PHE	2.5
1	B	578	ARG	2.5
1	B	707	LEU	2.4
1	A	743	ASN	2.4
1	A	405	GLY	2.4
1	B	745	ASN	2.4
1	A	668	THR	2.3
1	B	682	GLY	2.3
1	B	278	VAL	2.3
1	A	308	GLY	2.2
1	A	711	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	727	ASP	2.2
1	A	723	ARG	2.2
1	A	643	HIS	2.2
1	B	460	VAL	2.1
1	A	663	ILE	2.1
1	B	630	GLU	2.1
1	A	170	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

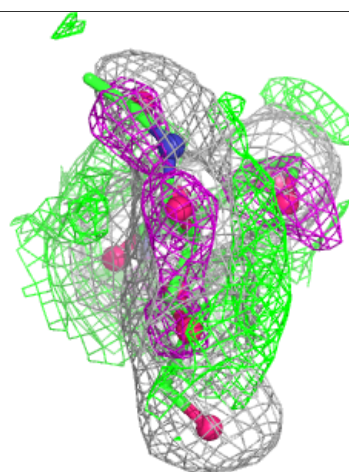
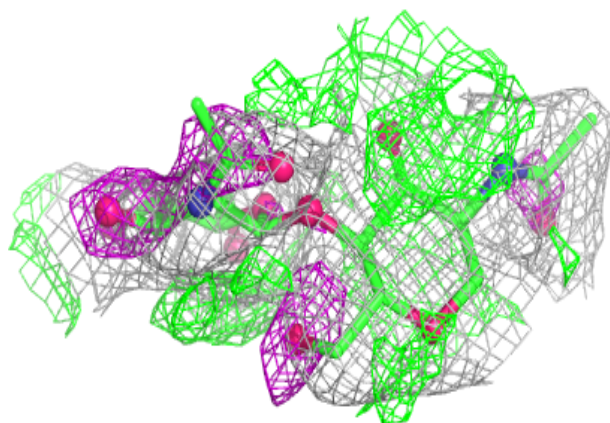
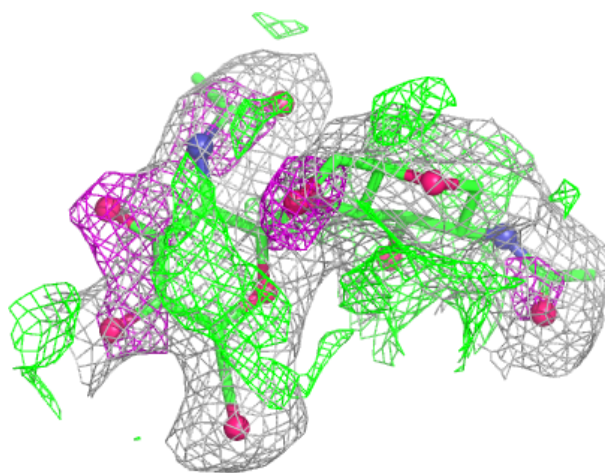
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	F	1	14/15	0.51	0.18	66,72,75,76	0
4	FUC	F	2	10/11	0.57	0.17	76,78,78,78	0
2	NAG	C	2	14/15	0.69	0.15	14,16,19,20	14
3	NAG	G	3	14/15	0.70	0.17	55,55,57,58	0
2	NAG	C	1	14/15	0.75	0.14	13,14,16,18	14
3	FUC	G	2	10/11	0.79	0.12	54,54,55,55	0
3	NAG	D	3	14/15	0.79	0.12	53,56,57,57	0
3	NAG	E	3	14/15	0.81	0.12	78,78,79,79	0
3	NAG	G	1	14/15	0.82	0.13	51,53,54,55	0
3	NAG	H	1	14/15	0.85	0.11	60,62,64,64	0
3	NAG	H	3	14/15	0.87	0.09	65,66,66,67	0
3	FUC	D	2	10/11	0.89	0.09	57,58,59,59	0
3	NAG	E	1	14/15	0.90	0.09	75,76,78,78	0
3	FUC	H	2	10/11	0.91	0.08	64,65,65,66	0
3	FUC	E	2	10/11	0.91	0.09	79,79,79,79	0
3	NAG	D	1	14/15	0.92	0.08	51,53,55,55	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

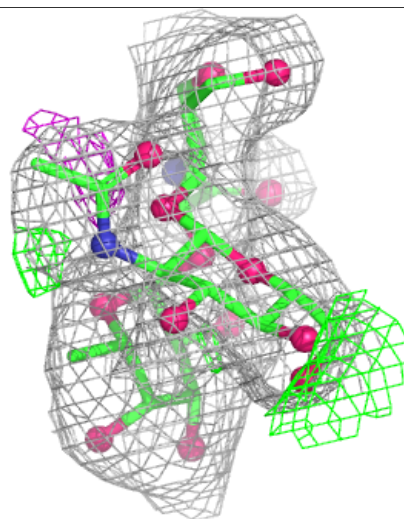
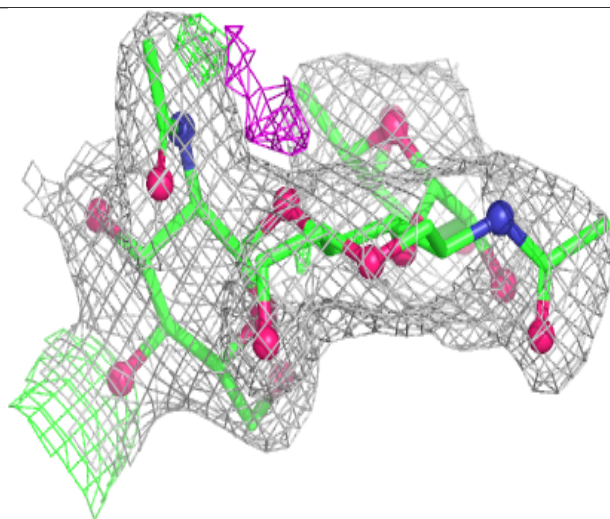
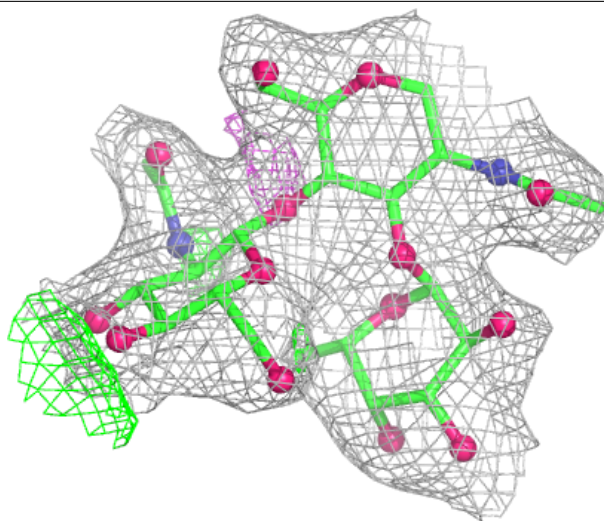
Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



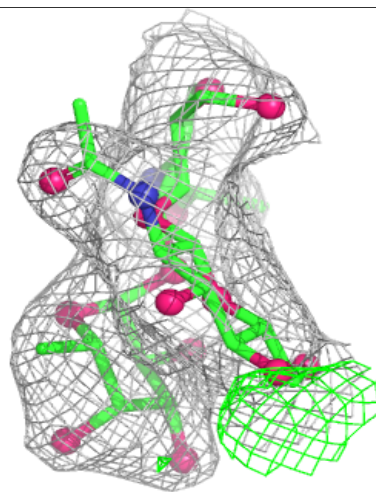
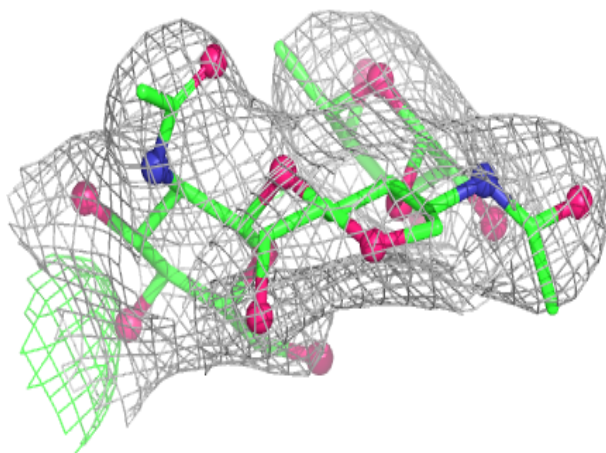
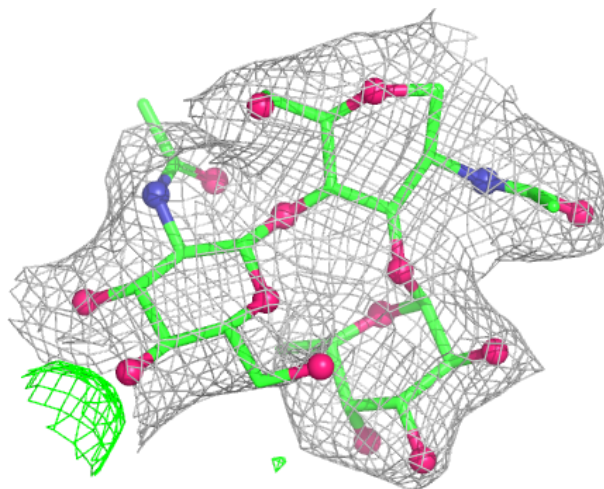
Electron density around Chain D:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



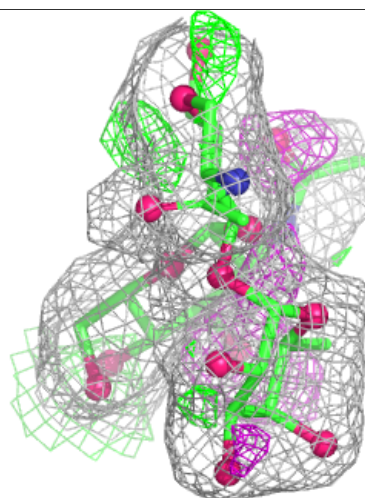
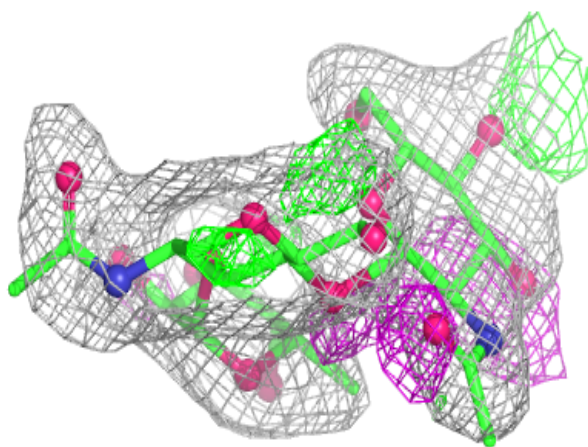
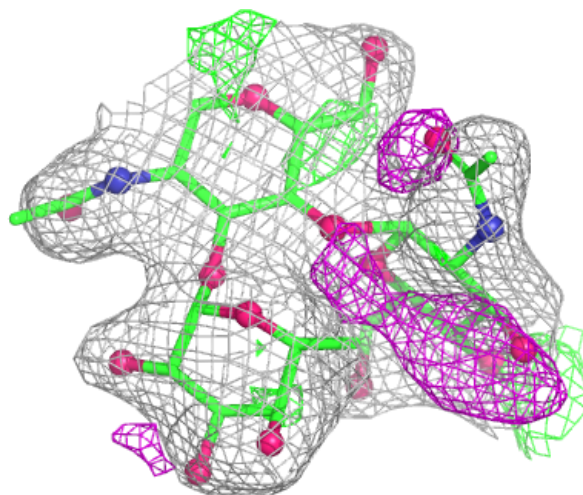
Electron density around Chain E:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



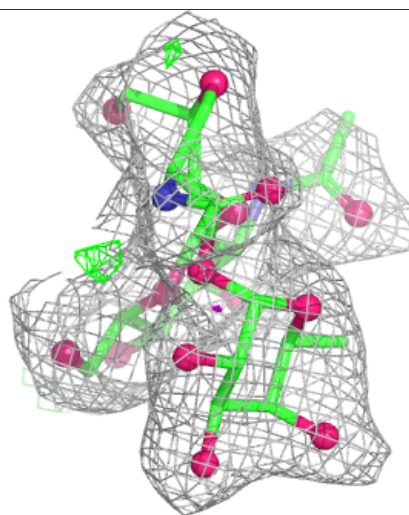
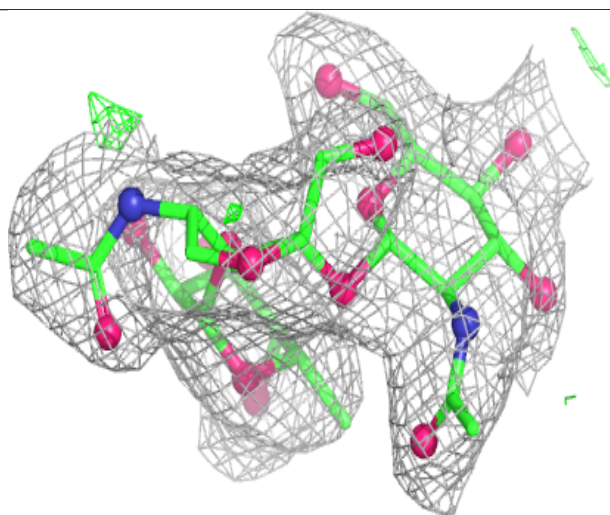
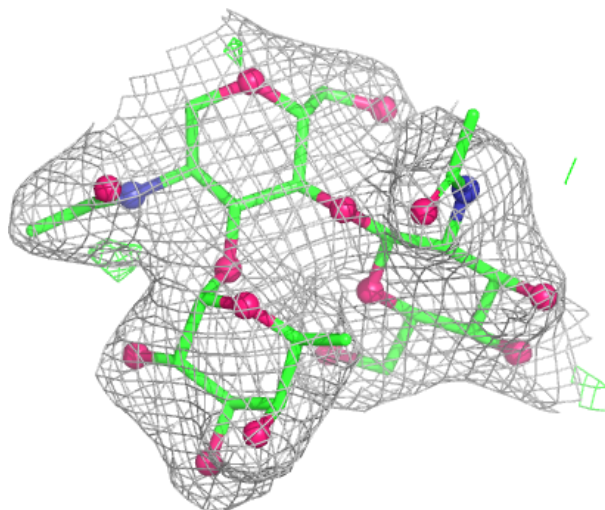
Electron density around Chain G:

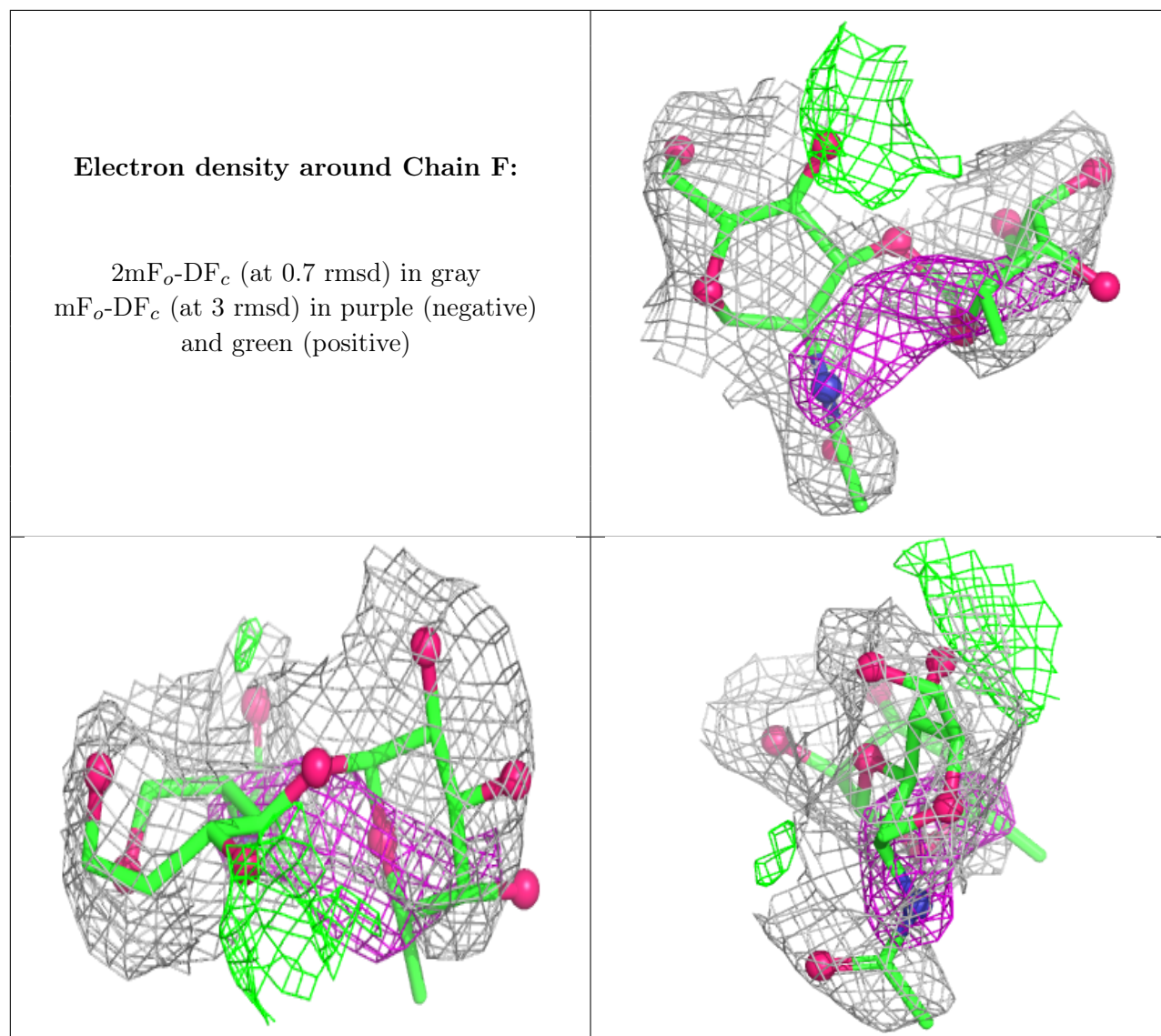
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.